Les valeurs finales des coordonnées atomiques et des coefficients d'agitation thermique équivalents sont consignées dans les Tableaux 1 et 2.*

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* Les listes des facteurs de structure et des facteurs d'agitation thermique anisotrope ont été déposées au dépôt d'archives de la British Library Document Supply Centre (Supplementary Publication No. SUP 51813: 19 pp.). On peut en obtenir des copies en s'adressant à: The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre.

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trans-Dichlorobis(cyclohexylamine)palladium(II)

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Abstract. $[PdCl_2(C_6H_{13}N)_2]$, $M_r = 375.68$, orthorhombic, *Pnca*, $a = 9.039$ (1), $b = 26.242$ (4), $c = 6.612$ (1) Å, $V = 1568.4$ (4) Å^3, $Z = 4$, $D_x = 1.59$ Mg m^{-3}, $\lambda(Mo\,K\alpha) = 0.71073$ Å, $\mu = 1.482$ mm^{-1}, $F(000) = 768$, $T = 298$ K, $R = 0.0219$ for 1473 observed reflections $[|F| > 3\sigma(F)]$. The complex molecule is the *trans* isomer of a square-planar structure, and the central Pd^{II} is coordinated by two Cl and two amino N atoms, lying on a center of symmetry.

Experimental. The title compound was prepared by refluxing a methanol solution of dichlorobis(dimethyl sulfoxide)palladium(II) (Price, Williamson, Schramm & Wayland, 1972) and cyclohexylamine at 323 K for 5 to 15 min and setting aside for 2 weeks. A yellow needle crystal with dimensions $0.44 \times 0.16 \times 0.08$ mm was used for X-ray diffractometry; Rigaku AFC-5R diffractometer, graphite-monochromated Mo $K\alpha$ radiation; cell dimensions from least-squares fit of 25 reflections with $25 < 2\theta < 30°$. Data collected by ω scans of 3° min^{-1} in ω; $2\theta_{max} = 60°$, h 0–12, k –36–36, l 0–9; no significant crystal movement or decay; numerical absorption correction based on Gaussian integration, minimum and maximum transmission factors 0.791, 0.890; 5511 reflections measured, 1473 independent reflections with $|F| > 3\sigma(F)$ observed, $R_{int} = 0.0155$ for 1348 symmetry-related pairs.

Structure solved by Patterson and Fourier methods; refined (on F) by a block-diagonal least-squares method, 131 parameters; H atoms included with isotropic thermal factors; $R = 0.0219$, $wR = 0.0305$, $S = 1.16$; $w = [\sigma_c^2 + (0.020\,|F_o|)^2]^{-1}$; max. (shift/$\sigma$) $= 0.3$; max., min. of ΔF synthesis 0.40 and -0.46 e Å^{-3}; atomic f for neutral Pd, Cl, N, C and spherical H, and anomalous-scattering corrections from *International Tables for X-ray Crystallography* (1974); all computer programs from *UNICS*III (Sakurai & Kobayashi, 1979) and *ORTEP* (Johnson, 1965).

Atomic parameters are given in Table 1,‡ and distances and angles are listed in Table 2. Fig. 1 shows the molecular structure with the atomic numbering scheme.

Related literature. The compound is one of a series of anticancer drugs of *cis*-dichlorodiamineplatinum(II) complexes (Rosenberg, VanCamp, Trosko & Mansour, 1969). Palladium(II) complexes were also found to possess such an activity (Inagaki & Kidani, 1978). One of the authors has synthesized various palladium(II) complexes such as $[PdCl(chexa)_2(dmso)]Cl$, $[PdCl-(cpen)_2(tmso)]Cl$, and others containing nucleic acid

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‡ Lists of structure factors, anisotropic thermal parameters, positional and isotropic thermal parameters of H atoms, and a packing diagram have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51821 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional coordinates* ($\times 10^5$ *for* Pd *and* Cl *atoms;* $\times 10^4$ *for other atoms) and equivalent isotropic thermal parameters for the non-*H *atoms*

$$B_{eq} = \tfrac{4}{3}\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	$B_{eq}(\text{Å}^2)$
Pd	0	0	0	1·9
Cl	4194 (7)	5501 (2)	26550 (8)	3·0
N	692 (2)	−558 (1)	1972 (3)	2·4
C(1)	217 (2)	−1100 (1)	1737 (3)	2·1
C(2)	1114 (3)	−1439 (1)	3119 (4)	2·5
C(3)	616 (3)	−1993 (1)	2918 (4)	3·1
C(4)	−1019 (3)	−2049 (1)	3345 (4)	3·3
C(5)	−1912 (3)	−1700 (1)	1987 (4)	3·1
C(6)	−1421 (2)	−1146 (1)	2166 (4)	2·5

Table 2. *Selected bond distances* (Å) *and angles* (°)

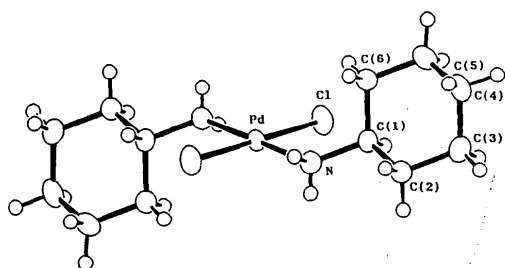| Pd–Cl	2·304 (1)	Cl–Pd–N	85·02 (6)
Pd–N	2·058 (2)	Pd–N–C(1)	121·6 (1)
N–C(1)	1·494 (3)	N–C(1)–C(2)	110·1 (2)
C(1)–C(2)	1·511 (3)	N–C(1)–C(6)	109·7 (2)
C(1)–C(6)	1·512 (3)	C(1)–C(2)–C(3)	110·5 (2)
C(2)–C(3)	1·528 (3)	C(2)–C(3)–C(4)	111·4 (2)
C(3)–C(4)	1·512 (4)	C(3)–C(4)–C(5)	110·6 (2)
C(4)–C(5)	1·516 (4)	C(4)–C(5)–C(6)	112·1 (2)
C(5)–C(6)	1·525 (3)	C(1)–C(6)–C(5)	110·2 (2)

Fig. 1. *ORTEP* drawing of the complex molecule with thermal ellipsoids at the 50% probability level.

bases, and discussed the structures (dmso = dimethyl sulfoxide, tmso = 2,5-dihydrothiophene 1-oxide, chexa = cyclohexylamine, cpen = cyclopentylamine) (Oh & Chung, 1985; Oh & Mo, 1986).

The authors are indebted to the IMS Japan–Korea Cooperation Program which enabled SOO to join the present joint research.

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Structure of Monoclinic Chloro(*meso*-tetraphenylporphyrinato)iron(III)

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Abstract. [FeCl(C$_{44}$H$_{28}$N$_4$)], $M_r = 704\cdot03$, monoclinic, $P2_1/n$, $a = 10\cdot254$ (2), $b = 15\cdot969$ (3), $c = 20\cdot810$ (4) Å, $\beta = 90\cdot48$ (2)°, $V = 3407\cdot7$ Å^3, $Z = 4$, $D_x = 1\cdot37$ g cm^{-3}, Mo $K\alpha$, $\bar{\lambda} = 0\cdot71073$ Å, $\mu = 5\cdot6$ cm^{-1}, $F(000) = 363$, $T = 293$ K, $R = 0\cdot047$ for 3357 unique observed reflections. The iron(III) ion is coordinated to a chloride, Fe—Cl $= 2\cdot211$ (1) Å, and four porphyrinato N atoms, average Fe—N $= 2\cdot070$ (9) Å. The iron(III) is displaced $0\cdot57$ Å from the mean plane of the 24-atom core.

Experimental. Crystals of the title compound were obtained in the course of an investigation of the reaction of nitrite ion with (*meso*-tetraphenylporphyrinato)-iron(III) (Finnegan, 1988). A deep-purple crystal 0·4 × 0·25 × 0·10 mm mounted on a glass fiber. Intensities measured with a Nicolet $P\bar{1}$ diffractometer using θ–2θ scans at a variable rate of 2–12° in 2θ to a maximum value of 55°. 60 reflections used for measuring lattice parameters, $21\cdot2 < \theta < 36\cdot4$°. Range of hkl: −11→12, 0→19, 0→24. 8420 reflections measured, 7581 unique, 3357 with $I > 3\sigma(I)$ considered observed. Merging R 0·035 for 199 duplicates. Four standard reflections, 2% intensity variation. No correction for absorption. Solved by Patterson and Fourier methods. Full-matrix least squares minimized $w(\Delta F)^2$ with a total of 451 variables. The H atoms were positioned according to idealized geometry (C—H