C(2)—C(4)	1.398 (5)	C(11)—C(14)	1.408 (6)
C(2)—N	1.323 (5)	C(12)—C(15)	1.387 (6)
C(3)—C(4)	1.423 (6)	C(13)—N	1.494 (5)
C(3)—C(5)	1.403 (5)	C(14)—C(16)	1.377 (5)
C(3)—C(6)	1.407 (5)	C(15)—C(17)	1.378 (6)
C(4)—C(9)	1.412 (5)	C(16)—C(17)	1.412 (5)
C(6)—C(7)	1.358 (6)	C(16)—O(2)	1.361 (5)
C(7)—C(8)	1.402 (6)	C(17)—O(1)	1.353 (5)
C(8)—C(9)	1.395 (5)	C(18)—O(2)	1.427 (6)
C(8)—O(4)	1.352 (5)	C(19)—O(3)	1.420 (1)
C(9)—O(3)	1.352 (5)	C(20)—O(4)	1.416 (6)
C(2)—C(4)—C(9)	121.5 (8)	C(1)—N—C(2)	122.4 (9)
C(1)—C(5)—C(3)	122.8 (8)	C(16)—O(2)—C(18)	116.0 (9)
C(3)—C(6)—C(7)	120.8 (8)	C(9)—O(3)—C(19)	120.2 (9)
C(6)—C(7)—C(8)	123.0 (1)	C(8)—O(4)—C(20)	119.3 (8)
C(7)—C(8)—O(4)	124.5 (9)	C(1)—C(11)—C(14)	120.0 (9)
C(7)—C(8)—C(9)	119.1 (8)	C(8)—C(9)—O(3)	125.0 (1)
C(9)—C(8)—O(4)	116.3 (8)	C(4)—C(9)—O(3)	117.0 (1)
C(4)—C(9)—C(8)	118.9 (7)	C(12)—C(10)—C(13)	110.8 (8)
C(10)—C(12)—C(15)	121.9 (8)	C(10)—C(12)—C(11)	118.6 (8)
C(10)—C(13)—N	111.7 (8)	C(12)—C(11)—C(14)	119.5 (9)
C(11)—C(14)—C(16)	120.6 (9)	C(11)—C(12)—C(15)	119.4 (8)
C(12)—C(15)—C(17)	122.0 (1)	C(1)—C(11)—C(12)	120.4 (8)
C(14)—C(16)—O(2)	126.0 (1)	C(11)—C(1)—N	118.6 (9)
C(14)—C(16)—C(17)	119.5 (8)	C(5)—C(1)—N	117.0 (9)
C(17)—C(16)—O(2)	115.5 (8)	C(5)—C(1)—C(11)	124.4 (7)
C(15)—C(17)—C(16)	119.4 (9)	C(4)—C(2)—N	122.3 (8)
C(16)—C(17)—O(1)	116.6 (8)	C(6)—C(3)—C(4)	118.3 (8)
C(15)—C(17)—O(1)	124.0 (9)	C(5)—C(3)—C(6)	123.8 (7)
C(2)—N—C(13)	118.8 (8)	C(5)—C(3)—C(4)	117.9 (8)
C(1)—N—C(13)	118.6 (8)	C(2)—C(4)—C(3)	117.6 (9)
C(3)—C(4)—C(9)—C(8)	−177.9	C(4)—C(9)—C(8)—C(7)	175.7
C(1)—C(5)—C(3)—C(4)	−178.9	C(9)—C(8)—C(7)—C(6)	−177.3
C(1)—N—C(2)—C(4)	−179.6	C(7)—C(6)—C(3)—C(4)	176.4
C(3)—C(4)—C(2)—N	179.3	N—C(1)—C(11)—C(12)	164.6
C(3)—C(5)—C(1)—N	178.7	N—C(13)—C(10)—C(12)	137.1
C(2)—C(4)—C(3)—C(5)	180.0	C(11)—C(1)—N—C(13)	174.8
C(2)—N—C(1)—C(5)	−179.4	C(11)—C(12)—C(10)—C(13)	−141.1
C(6)—C(3)—C(4)—C(9)	−178.2	C(8)—C(7)—C(6)—C(3)	−178.6
C(1)—N—C(13)—C(10)	−141.1	C(1)—C(11)—C(12)—C(10)	179.3
C(11)—C(12)—C(15)—C(17)	−179.2	C(11)—C(14)—C(16)—C(17)	−179.4
C(12)—C(15)—C(17)—C(16)	179.1	C(12)—C(11)—C(14)—C(16)	179.4
C(14)—C(16)—C(17)—C(15)	−179.8	C(14)—C(11)—C(12)—C(15)	179.9

The structure was solved by direct and Fourier methods: *SHELXS*86 (Sheldrick, 1986) used with 304 *E*'s > 1.2. Most of the C atoms were located from the best *E* map. A subsequent difference Fourier map based on these atoms revealed the rest of the non-H atoms in the asymmetric unit. The structure was refined by full-matrix least squares using *SHELX*76 (Sheldrick, 1976).

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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71129 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CD1033]

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5,10,15,20-Tetrakis(*p*-chlorophenyl)-porphyrin

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Abstract

The title molecule, 2,7,12,17-tetrakis(4-chlorophenyl)-21,22,23,24-tetraazapentacyclo[16.2.1.$1^{3,6}$.$1^{8,11}$.$1^{13,16}$]tetracosa-1,3(22),4,6,8,10,12,14,16(24),17,19-undecaene, is crystallographically centrosymmetric and the dihedral angle between the two pyrrole ring planes is 5.0 (4)°. The molecular structure is a consequence of steric hinderances between the α-H atoms of the pyrrole and the *ortho*-H atoms of the phenyl rings. The dihedral angles between the pyrrole and phenyl rings are 54.8 (4) and 111.1 (3)°, respectively. The sums of the angles around *meso*-C atoms are 360° and the average bond length between *meso* and adjacent macrocyclic ring C atoms is 1.398 (6) Å.

Comment

Porphyrins and their metal complexes are used as catalysts (Ostovic & Bruice, 1989), photosensitizers (Milgrom, 1984; Davila & Harriman, 1990) or useful synthetic precursors to mono-oxygenase and allosteric enzyme model systems (Tabushi & Kugimiya, 1986). The substituents in porphyrins, bonded to *meso*-C atoms, are effective in forming metal complexes (Ulman, Fisher & Ibers, 1982).

The X-ray crystallographic structure determinations of some synthetic free-base porphyrins have been reported, *e.g.* porphine (Chen & Tulinsky, 1972), tetraphenyl porphyrin (TPP) (Silvers & Tulinsky, 1967) and tetra-*n*-propylporphyrin

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(Codding & Tulinsky, 1972). The structure determination of the title compound was undertaken to elucidate the effects of steric interactions on the bond lengths and angles concerned. The title compound, subsequently denoted H_2(*p*-ClTPP), was prepared from *p*-chlorobenzaldehyde and pyrrole by the Lindsey method using boron trifluoride etherate as catalyst (Lindsey, Schreiman, Hsu, Kearney & Marguerettaz, 1987; Lindsey & Wagner, 1989).

A view of the molecule and the atomic numbering are shown in Fig. 1; a view of the crystal packing is shown in Fig. 2. H_2(*p*-ClTPP) has a symmetry centre. The fact that H atoms are bonded to N1 and N1*B*, but not to N2 and N2*B*, indicates that the pyrroles differ from one another in the different pairs, similar to triclinic TPP (Silvers & Tulinsky, 1967). The distances between neighbouring phenyl and pyrrole H atoms [H3···H9 2.985 (8), H5···H21*B* 2.829 (8), H10···H14 2.757 (7), H18···H20 2.906 (8) Å] and the close van der Waals contact between the pyrrole (N)H atoms [H1···H1*B* 2.156 (5) Å], cause a great deal of steric crowding. These steric effects tilt the *p*-chlorophenyl groups out of the molecular plane. Deviations from perpendicularity of the porphine and *p*-chlorophenyl rings can be correlated with the degree of planarity of porphine ring. The *p*-chlorophenyl rings seem to be rotated considerably out of the plane of the macrocycle. An examination of the deviations from the individual pyrrole and phenyl least-sqaures planes shows that the rings *B* (N1, C8, C9, C10, C11), *C* (C13, C14, C15, C16, C17, C18) and *D* (N2, C19, C20, C21, C22) are planar [the maximum distances to the least-squares plane are 0.028 (5), −0.016 (6) and −0.019 (6) Å, respectively], while ring *A* (C1, C2, C3, C4, C5, C6) is not planar [maximum deviation of C6 −0.687 (8) Å from the least-squares plane]. The rings are also twisted with respect to each other. The porphine nucleus *E* (C7, C8, N1, C11, C12, C19, N2, C22, C7*B*, C8*B*, N1*B*, C11*B*, C12*B*, C19*B*, N2*B*, C22*B*) is non-planar [maximum deviation of C22*B* 1.118 (5) Å from the least-squares plane]. The dihedral angles between the least-squares planes are *A*—*B* 54.8 (4), *A*—*C* 89.7 (2), *A*—*D* 52.2 (4), *A*—*E* 65.4 (3), *B*—*C* 111.1 (3), *B*—*D* 5.0 (4), *B*—*E* 13.3 (3), *C*—*D* 106.3 (4), *C*—*E* 121.8 (2) and *D*—*E* 18.1 (4)°.

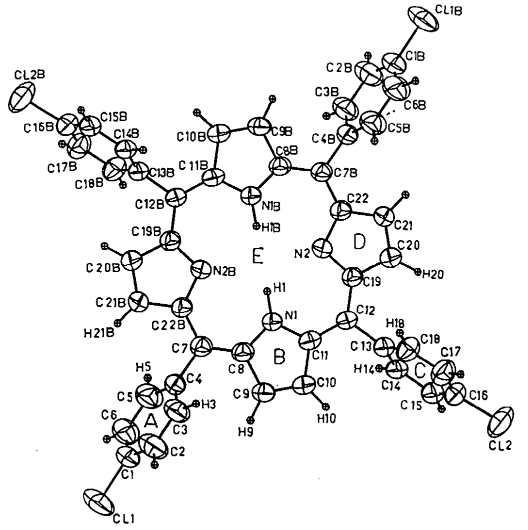

Fig. 1. *SNOOPI* (Davies, 1983) drawing of the title molecule with the atom-numbering scheme. The thermal ellipsoids are drawn at the 50% probability level.

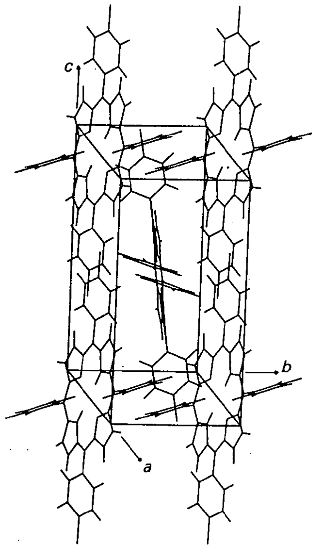

Fig. 2. The overall packing diagram of the molecule.

Deviations from planarity in the porphine nucleus are probably the result of repulsion effects arising from the close contacts between the nearest H atoms of the phenyl and pyrrole rings, as well as between H1 and H1*B*. It is greatly increased when the molecules are packed closely in the crystals. Organic molecules tend to pack in crystals as closely as their geometry allows (Kitaigorodskii, 1955). The porphine nucleus will remain planar, if possible, in order to increase overlap of π orbitals. When there are substituents bent at a sharp angle to the porphine nucleus, the molecules cannot be close packed and remain planar at the same time (Fleischer, Miller & Webb, 1964). Consequently, the shape of a particular porphyrin in a crystal appears to depend on the substituents and the type of packing. The behaviour of the bond angles of the two different pyrroles shows that the N—H bonded pyrrole undergoes changes arising from repulsion of atoms H1 and H1*B*, which results in an increase of the C8—N1—C11 angle [109.2 (3)°]. In addition, the C19—N2—C22 angle [106.1 (3)°] is 3.1 (3)° less than the C8—N1—C11 angle. The bond lengths and angles around C atoms on pyrrole rings are affected to a lesser extent. The average C—N1 distance is 1.370 (6) Å as compared to the average C—N2 distance of 1.379 (6) Å. The average C—C bond distances in the two phenyl rings (*A* and *C*) are 1.370 (8) and 1.387 (7) Å, respectively.

The optimum value for the diameter of the hole of triclinic TPP (Silvers & Tulinsky, 1967) and an undistorted porphyrin complex (Shachter, Fleischer & Haltiwanger, 1987; Scheidt, Mondal, Eigenbrot, Adler, Radonovich & Hoard, 1986) has been estimated as 4.06 Å. In H_2(*p*-ClTPP), the N2···N2*B* distance [4.060 (5) Å] is smaller than the N1···N1*B* distance [4.154 (5) Å]. Numerous porphyrin complexes have been synthesized (Robinson & Hambright, 1991); the porphyrin cores are, in general, non-planar and can be further distorted when the porphyrin molecules accommodate metal cations that are larger or smaller than the central holes. These distortions are referred to as 'doming' and 'ruffling', respectively (Hoard, 1975). As mentioned above, the diameter of the hole in the title molecule has now been specified, which will be helpful for the preparation of metal complexes.

Experimental

Crystal data

$C_{44}H_{26}Cl_4N_4$
M_r = 752.53
Monoclinic
$P2_1/a$
a = 15.776 (13) Å
b = 8.646 (3) Å
c = 14.087 (5) Å
β = 96.05 (5)°
V = 1910.7 (3) Å^3
Z = 2
D_x = 1.308 Mg m^{-3}

Cu $K\alpha$ radiation
λ = 1.54180 Å
Cell parameters from 25 reflections
θ = 6–16°
μ = 6.30 mm^{-1}
T = 293 K
Plate
1.0 × 0.6 × 0.15 mm
Purple

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
5269 measured reflections
3638 independent reflections
2259 observed reflections [$F \geq 3\sigma(F)$]

$\theta_{\max}$ = 75°
$h = -19 \rightarrow 18$
$k = 0 \rightarrow 10$
$l = 0 \rightarrow 17$
3 standard reflections
frequency: 180 min
intensity variation: 1%

Refinement

Refinement on F
Final R = 0.070
wR = 0.088
1890 reflections
235 parameters
H-atom parameters not refined

$(\Delta/\sigma)_{\max}$ = 0.00
$\Delta\rho_{\max}$ = 0.94 e Å^{-3}
$\Delta\rho_{\min}$ = −1.95 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

U_{eq} is the mean of the principal axes of the thermal ellipsoid.

	x	y	z	U_{eq}
C1	0.1618 (4)	0.2750 (10)	0.0080 (4)	0.0093 (3)
C2	0.1618 (4)	0.3690 (10)	0.9309 (4)	0.0092 (3)
C3	0.1330 (4)	0.3150 (8)	0.8412 (4)	0.0073 (2)
C4	0.1029 (3)	0.1664 (7)	0.8276 (3)	0.0054 (2)
C5	0.1044 (4)	0.0742 (8)	0.9074 (4)	0.0077 (3)
C6	0.1330 (4)	0.1270 (10)	0.9968 (4)	0.0096 (3)
C7	0.0729 (3)	0.1109 (6)	0.7299 (3)	0.0051 (1)
C8	0.1329 (3)	0.0949 (6)	0.6655 (3)	0.0051 (2)
C9	0.2238 (3)	0.1210 (6)	0.6858 (3)	0.0054 (2)
C10	0.2596 (3)	0.1031 (6)	0.6037 (3)	0.0054 (2)
C11	0.1933 (3)	0.0626 (6)	0.5305 (3)	0.0048 (1)
C12	0.2035 (3)	0.0359 (6)	0.4350 (3)	0.0049 (1)
C13	0.2910 (3)	0.0564 (6)	0.4048 (3)	0.0049 (1)
C14	0.3570 (3)	−0.0455 (6)	0.4330 (3)	0.0051 (2)
C15	0.4370 (3)	−0.0283 (7)	0.4017 (3)	0.0060 (2)
C16	0.4512 (3)	0.0924 (7)	0.3427 (4)	0.0064 (2)
C17	0.3878 (3)	0.1967 (7)	0.3143 (4)	0.0070 (2)
C18	0.3081 (3)	0.1793 (7)	0.3451 (4)	0.0063 (2)
C19	0.1387 (3)	−0.0095 (6)	0.3638 (3)	0.0048 (1)
C20	0.1526 (3)	−0.0502 (7)	0.2685 (3)	0.0057 (2)
C21	0.0769 (3)	−0.0967 (7)	0.2231 (3)	0.0059 (2)
C22	0.0144 (3)	−0.0799 (6)	0.2904 (3)	0.0051 (2)
N1	0.1177 (2)	0.0587 (5)	0.5710 (2)	0.0048 (1)
N2	0.0541 (2)	−0.0289 (5)	0.3767 (2)	0.0049 (1)
Cl1	0.1994 (2)	0.3420 (4)	0.1207 (1)	0.0163 (3)
Cl2	0.5496 (9)	0.1143 (3)	0.2996 (1)	0.0105 (3)

Table 2. *Geometric parameters* (Å, °)

C1—Cl1	1.735 (6)	C11—C12	1.391 (6)
C1—C2	1.360 (10)	C12—C13	1.498 (6)
C1—C6	1.360 (10)	C12—C19	1.410 (6)
C2—C3	1.377 (7)	C13—C14	1.389 (6)
C3—C4	1.376 (8)	C13—C18	1.400 (7)
C4—C5	1.376 (7)	C14—C15	1.389 (7)
C4—C7	1.488 (6)	C15—C16	1.367 (8)
C5—C6	1.369 (8)	C16—Cl2	1.736 (14)
C7—C22*B*	1.404 (6)	C16—C17	1.374 (8)
C7—C8	1.385 (6)	C17—C18	1.380 (7)
C8—C9	1.450 (6)	C19—C20	1.427 (6)
C8—N1	1.364 (6)	C19—N2	1.377 (5)
C9—C10	1.349 (7)	C20—C21	1.354 (7)
C10—C11	1.433 (6)	C21—C22	1.445 (6)
N1—C11	1.375 (5)	C22—N2	1.380 (6)
Cl1—C1—C2	120.2 (7)	C11—C12—C13	117.4 (4)
Cl1—C1—C6	119.9 (6)	C13—C12—C19	116.8 (4)
C2—C1—C6	119.9 (6)	C12—C13—C14	121.9 (5)
C1—C2—C3	120.3 (7)	C12—C13—C18	120.2 (4)
C2—C3—C4	121.2 (6)	C14—C13—C18	117.9 (4)
C3—C4—C5	116.8 (5)	C13—C14—C15	121.3 (5)
C3—C4—C7	120.1 (4)	C14—C15—C16	119.2 (5)
C5—C4—C7	123.1 (5)	C15—C16—C17	121.1 (5)
C4—C5—C6	122.4 (7)	Cl2—C16—C15	120.4 (4)
C1—C6—C5	119.4 (6)	Cl2—C16—C17	118.5 (5)
C4—C7—C8	117.8 (4)	C16—C17—C18	119.8 (6)
C4—C7—C22*B*	117.3 (4)	C13—C18—C17	120.7 (5)
C8—C7—C22*B*	124.9 (4)	N2—C19—C12	125.4 (4)
N1—C8—C7	126.9 (4)	N2—C19—C20	110.0 (4)
N1—C8—C9	107.2 (4)	C12—C19—C20	124.5 (4)
C7—C8—C9	125.8 (4)	C19—C20—C21	107.6 (4)
C8—C9—C10	107.9 (4)	C20—C21—C22	106.8 (4)
C9—C10—C11	107.7 (4)	N2—C22—C7*B*	125.7 (4)
N1—C11—C10	107.9 (4)	N2—C22—C21	109.5 (4)
N1—C11—C12	126.2 (4)	C7*B*—C22—C21	124.8 (4)
C10—C11—C12	125.8 (4)	C8—N1—C11	109.2 (3)
C11—C12—C19	125.8 (4)	C19—N2—C22	106.1 (3)

H atoms were geometrically positioned 1.0 Å from the corresponding atoms and a riding model was used in the refinement process. Initially, a unit weighting scheme was used, but in the final stages of the refinement the weights were assigned using the method described by Carruthers & Watkin (1979), as incorporated in the *CRYSTALS* program package (Watkin, Carruthers & Betteridge, 1985). Programs used were *CRYSTALS*, *SHELXS*86 (Sheldrick, 1986) and *SNOOPI* (Davies, 1983).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and bond distances and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71143 (18 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AB1038]

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Structure of 5-[1-(Diaminomethylenehydrazono)ethyl]-4-methyl-2-methylthiopyrimidine

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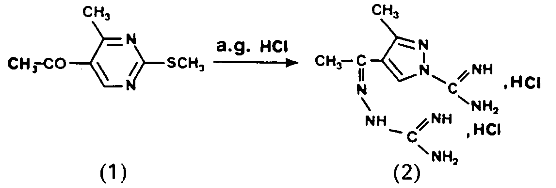
Abstract

The detailed structure of the title compound (5-acetyl-4-methyl-2-methylthiopyrimidine diaminomethylenehydrazone) revealed distinct differences between it and its already published dichloride salt. It is obviously characterized by its diaminomethylenehydrazono chain and the more symmetrical pyrimidine ring. This observation helps in understanding the chemical behavior of the molecule and sheds more light on the possible mechanism of action of antitumor drugs such as mitoguazone.

Comment

5-Acetyl-4-methyl-2-methylthiopyrimidine (1) is transformed by aminoguanidine hydrochloride (a.g. HCl) in acidic boiling methanol into 4-acetyl-1-amidino-3-methylpyrazole amidinohydrazone dihydrochloride (2) (Menichi, Naciri, Kokel & Hubert-Habart, 1984).



(1) (2)

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