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2,3,12,13-Tetramethyl-5,10,15,20-tetraphenylporphyrin

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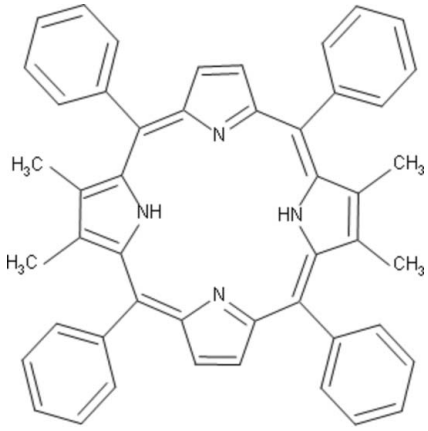
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.076; wR factor = 0.165; data-to-parameter ratio = 21.6.

In the crystal structure of the title compound, $C_{48}H_{38}N_4$, the molecule is positioned on a center of symmetry and the porphyrin ring shows a nearly planar geometry in spite of the presence of four bulky methyl groups at the antipodal β-pyrrole positions.

Related literature

For related crystal structures, see: Bhyrappa *et al.* (2006); Scheidt (2000); Scheidt & Lee (1987); Senge (2000); Shelnutt *et al.* (1998); Silvers & Tulinsky (1967); Zou *et al.* (1995); Terazono *et al.* (2002).



Experimental

Crystal data

$C_{48}H_{38}N_4$
M_r = 670.82
Monoclinic, $P2_1/n$
a = 13.5507 (3) Å
b = 6.7094 (1) Å
c = 19.4638 (4) Å
β = 102.463 (1)°
V = 1727.89 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 (2) K
0.30 × 0.22 × 0.19 mm

Data collection

Bruker Kappa APEX2 diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.910, T_{max} = 0.986
26484 measured reflections
5108 independent reflections
3353 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.165
S = 1.04
5108 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Sheldrick, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2056).

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supplementary materials

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2,3,12,13-Tetramethyl-5,10,15,20-tetraphenylporphyrin

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Comment

Structural aspects of porphyrins and metalloporphyrins are of continued interest due to their biological significance. The stereochemical features of porphyrin ring can be altered by the presence of peripheral substituents and also by core metal ions (Senge, 2000; Scheidt & Lee, 1987). Many structural reports are available on the structural properties of the porphyrins (Senge, 2000). The synthetic analogues have been employed as model compounds to mimic nonplanar porphyrins in nature (Shelnutt *et al.*, 1998).

The β–pyrrole substituted porphyrins are of growing interest because of their unique physicochemical properties. It was shown earlier that the five coordinated Zn(II)–complexes of 2,3,12,13–tetrabromo– (or tetramethyl)–5,10,15,20–tetraphenylporphyrin showed considerable nonplanarity of the porphyrin ring (Terazono *et al.*, 2003). However, free base tetrabromoporphyrin (H_2*TPP*Br_4) showed nearly planar structure (Zou *et al.*, 1995). To examine the role of β–tetrametylation on the stereochemical features of the porphyrin ring, we have examined the crystal structure of 2,3,12,13–tetramethyl–5,10,15,20–tetraphenylporphyrin, H_2*TPP*$(CH_3)_4$ (Fig. 1). This showed interesting structural features relative to the Zn*TPP*$CH_3)_4(C_4H_8O)_{1.6}(CHCl_3)_{0.4}$ structure (Terazono *et al.*, 2003).

The title compound (I) is positioned at the center of symmetry (Fig. 1). The C–C bond lengths of the porphyrin ring are comparable to the reported for H_2*TPP* (Silvers & Tulinsky, 1967) and Zn*TPP*$(CH_3)_4$ $(C_4H_8O)_{1.6}(CHCl_3)_{0.4}$ structures (Terazono *et al.*, 2003). Interestingly, the C–C distances of the β–pyrrole with β–methyl groups are found to be 1.369 (2)Å while the other β–pyrrole C–C distance was found to be 1.345 (2) Å. This is possibly due to steric effects rather than the electronic effect of the substituents (Scheidt, 2000). The increase in the core (N_4H_2) inter–nitrogen distances along the β–methyl substituted pyrrole is 4.341Å and the other opposite pyrroles is 3.960 Å. The average distance 4.150Å is similar to that reported for H_2*TPP*Br_4 (4.15 Å) (Zou *et al.*, 1995) and comparable to the reported values for H_2*TPP* (4.20 Å) structure (Silvers & Tulinsky, 1967). The elongation the core along the methyl substituted antipodal direction is presumably due to the enhanced steric crowding. Carbon atoms of the methyl groups on the given pyrrole groups are displaced from each other by 0.306 (4) Å. The mean plane deviation of the 24 atom ($C_{20}N_4$) core shows that the macrocyclic ring is nearly planar within 0.119 (4) Å. The observed nonplanarity of the ring is quite comparable to that reported for H_2*TPP*Br_4. The *meso*–phenyl rings are nearly planar with an average dihedral angle of 77.25 (5)° relative the mean plane.

Molecular packing diagram (Fig. 2) of the H_2*TPP*$(CH_3)_4$ shows interesting features. The molecules are arranged in a slipped stack orientation with a corrugated structure type arrangement. The inter porphyrin ring planes in column 1 and column 2 are oriented at an angle of 45° to each other. The closest inter–porphyrin distance between the core N_2 with the phenyl hydrogen distance is 2.743 Å. The porphyrins are held together largely by weak van der Waals forces.

Experimental

The title compound was prepared using the modified procedure for the synthesis of 2,3,5,10,12,13,15,20–octaphenylporphyrin (Bhyrappa *et al.*, 2006) employing excess of super base (40 mmol) and the reaction was completed in 12 h with 50% yield of the $H_2TPP(CH_3)_4$ derivative. The product was characterized by electronic absorption, proton NMR and mass Spectroscopic methods. The observed values are in agreement with the reported data (Bhyrappa *et al.*, 2006). The crystals of $H_2TPP(CH_3)_4$ were grown by vapour diffusion of methanol into a 1,1,2,2–tetrachloroethane solution of the porphyrin over a period of 3 days.

Figures

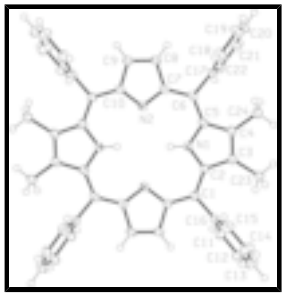

Fig. 1. Molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at 50% probability level. H atoms are presented as a spheres of arbitrary radius.

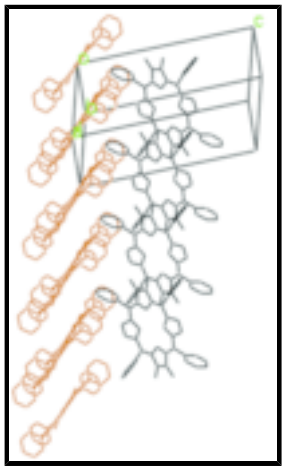

Fig. 2. The crystal packing diagram of the title compound, showing view in between a and c axes of the unit cell. Only two columns are shown in different colours. Hydrogen atoms are omitted for clarity.

2,3,12,13-Tetramethyl-5,10,15,20-tetraphenylporphyrin

Crystal data

$C_{48}H_{38}N_4$	F_{000} = 708
M_r = 670.82	D_x = 1.289 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5867 reflections
a = 13.5507 (3) Å	θ = 3.1–30.4°
b = 6.7094 (1) Å	μ = 0.08 mm^{-1}
c = 19.4638 (4) Å	T = 173 (2) K

β = 102.463 (1)º	Needle, black
V = 1727.89 (6) Å^3	0.30 × 0.22 × 0.19 mm
Z = 2	

Data collection

Bruker Kappa APEX2 diffractometer	5108 independent reflections
Radiation source: Fine–focus sealed tube	3353 reflections with $I > 2\sigma(I)$
Monochromator: Graphite	R_{int} = 0.051
T = 173(2) K	θ_{max} = 30.4º
ω– and φ–scan	θ_{min} = 2.1º
Absorption correction: multi-scan (Blessing, 1995)	h = −18→18
T_{min} = 0.910, T_{max} = 0.986	k = −9→8
26484 measured reflections	l = −27→27

Refinement

Refinement on F^2	Secondary atom site location: Difmap
Least-squares matrix: Full	Hydrogen site location: Geom
$R[F^2 > 2\sigma(F^2)]$ = 0.076	H-atom parameters constrained
$wR(F^2)$ = 0.165	$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 2.1167P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
5108 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
237 parameters	$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Primary atom site location: Direct	Extinction correction: None

Special details

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 $F^2 > 2\sigma(F^2)$ 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}
N1	0.12260 (12)	0.7865 (2)	0.02441 (8)	0.0196 (4)
H1	0.0765	0.8767	0.0161	0.023*
N2	−0.07612 (12)	0.8566 (2)	0.06079 (8)	0.0195 (4)

C1	0.22546 (15)	0.9211 (3)	−0.05388 (10)	0.0200 (4)
C2	0.20639 (15)	0.7816 (3)	−0.00481 (10)	0.0195 (4)
C3	0.26399 (15)	0.6072 (3)	0.02301 (10)	0.0214 (4)
C4	0.21183 (15)	0.5106 (3)	0.06600 (10)	0.0208 (4)
C5	0.12308 (15)	0.6273 (3)	0.06860 (10)	0.0195 (4)
C6	0.05040 (15)	0.5931 (3)	0.10860 (10)	0.0194 (4)
C7	−0.04024 (15)	0.6994 (3)	0.10417 (10)	0.0200 (4)
C8	−0.10803 (16)	0.6560 (3)	0.15066 (11)	0.0242 (4)
H8	−0.1000	0.5566	0.1847	0.029*
C9	−0.18473 (16)	0.7874 (3)	0.13498 (11)	0.0248 (5)
H9	−0.2402	0.7956	0.1559	0.030*
C10	−0.16427 (15)	0.9134 (3)	0.07928 (10)	0.0202 (4)
C11	0.39915 (16)	0.9993 (3)	−0.07463 (12)	0.0291 (5)
H11	0.4059	1.1002	−0.0412	0.035*
C12	0.47621 (18)	0.9645 (4)	−0.10983 (13)	0.0365 (6)
H12	0.5341	1.0430	−0.1001	0.044*
C13	0.46756 (19)	0.8153 (4)	−0.15890 (13)	0.0384 (6)
H13	0.5199	0.7916	−0.1819	0.046*
C14	0.3811 (2)	0.7004 (4)	−0.17410 (13)	0.0408 (6)
H14	0.3751	0.5989	−0.2073	0.049*
C15	0.30327 (18)	0.7368 (4)	−0.13965 (12)	0.0327 (5)
H15	0.2445	0.6611	−0.1507	0.039*
C16	0.31201 (15)	0.8843 (3)	−0.08904 (11)	0.0219 (4)
C17	0.07279 (15)	0.4411 (3)	0.16629 (10)	0.0197 (4)
C18	0.02474 (17)	0.2577 (3)	0.16021 (12)	0.0286 (5)
H18	−0.0191	0.2231	0.1182	0.034*
C19	0.04162 (19)	0.1250 (3)	0.21637 (12)	0.0337 (5)
H19	0.0090	0.0022	0.2119	0.040*
C20	0.10670 (18)	0.1752 (3)	0.27879 (12)	0.0316 (5)
H20	0.1171	0.0875	0.3167	0.038*
C21	0.15666 (17)	0.3576 (3)	0.28479 (11)	0.0279 (5)
H21	0.2018	0.3905	0.3264	0.034*
C22	0.13942 (15)	0.4895 (3)	0.22923 (11)	0.0228 (4)
H22	0.1725	0.6118	0.2337	0.027*
C23	0.36781 (17)	0.5402 (3)	0.01099 (12)	0.0286 (5)
H23A	0.4000	0.4556	0.0490	0.043*
H23B	0.4093	0.6551	0.0090	0.043*
H23C	0.3587	0.4682	−0.0325	0.043*
C24	0.23962 (17)	0.3052 (3)	0.09900 (11)	0.0247 (4)
H24A	0.2922	0.2474	0.0794	0.037*
H24B	0.1812	0.2203	0.0893	0.037*
H24C	0.2628	0.3192	0.1490	0.037*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0208 (8)	0.0188 (8)	0.0197 (8)	0.0029 (6)	0.0058 (7)	0.0037 (7)
N2	0.0215 (8)	0.0186 (8)	0.0180 (8)	0.0003 (7)	0.0037 (7)	0.0020 (7)

C1	0.0209 (10)	0.0212 (10)	0.0175 (10)	−0.0002 (8)	0.0035 (8)	0.0005 (8)
C2	0.0219 (10)	0.0199 (10)	0.0161 (9)	0.0018 (8)	0.0029 (8)	−0.0005 (8)
C3	0.0248 (10)	0.0218 (10)	0.0168 (10)	0.0034 (8)	0.0027 (8)	−0.0008 (8)
C4	0.0262 (10)	0.0191 (9)	0.0162 (9)	0.0029 (8)	0.0025 (8)	−0.0012 (8)
C5	0.0237 (10)	0.0183 (9)	0.0151 (9)	0.0000 (8)	0.0014 (8)	0.0007 (8)
C6	0.0237 (10)	0.0160 (9)	0.0173 (9)	−0.0016 (8)	0.0020 (8)	0.0011 (8)
C7	0.0237 (10)	0.0188 (9)	0.0173 (9)	−0.0028 (8)	0.0037 (8)	0.0011 (8)
C8	0.0254 (10)	0.0236 (10)	0.0239 (11)	−0.0018 (8)	0.0063 (8)	0.0089 (9)
C9	0.0236 (10)	0.0268 (11)	0.0254 (11)	−0.0025 (8)	0.0085 (9)	0.0059 (9)
C10	0.0216 (10)	0.0206 (10)	0.0180 (10)	−0.0019 (8)	0.0036 (8)	0.0023 (8)
C11	0.0268 (11)	0.0278 (11)	0.0330 (12)	−0.0015 (9)	0.0073 (9)	−0.0021 (9)
C12	0.0257 (12)	0.0422 (14)	0.0439 (14)	−0.0032 (10)	0.0126 (11)	0.0038 (12)
C13	0.0343 (13)	0.0495 (15)	0.0366 (14)	0.0052 (11)	0.0193 (11)	0.0027 (12)
C14	0.0456 (15)	0.0483 (16)	0.0338 (13)	−0.0005 (12)	0.0202 (12)	−0.0103 (12)
C15	0.0336 (12)	0.0368 (13)	0.0302 (12)	−0.0076 (10)	0.0125 (10)	−0.0054 (10)
C16	0.0228 (10)	0.0233 (10)	0.0200 (10)	0.0021 (8)	0.0059 (8)	0.0048 (8)
C17	0.0218 (10)	0.0195 (9)	0.0183 (10)	0.0023 (8)	0.0053 (8)	0.0033 (8)
C18	0.0332 (12)	0.0239 (11)	0.0257 (11)	−0.0047 (9)	−0.0004 (9)	0.0026 (9)
C19	0.0427 (14)	0.0225 (11)	0.0339 (13)	−0.0066 (10)	0.0041 (11)	0.0077 (10)
C20	0.0401 (13)	0.0301 (12)	0.0250 (12)	0.0074 (10)	0.0075 (10)	0.0126 (10)
C21	0.0295 (11)	0.0336 (12)	0.0177 (10)	0.0074 (9)	−0.0016 (9)	−0.0011 (9)
C22	0.0239 (10)	0.0217 (10)	0.0230 (10)	−0.0008 (8)	0.0053 (8)	−0.0013 (8)
C23	0.0405 (13)	0.0228 (11)	0.0261 (11)	0.0095 (9)	0.0151 (10)	0.0054 (9)
C24	0.0306 (11)	0.0230 (10)	0.0213 (10)	0.0034 (9)	0.0074 (9)	0.0008 (8)

Geometric parameters (Å, °)

N1—C5	1.370 (2)	C12—C13	1.371 (4)
N1—C2	1.376 (3)	C12—H12	0.9300
N1—H1	0.8600	C13—C14	1.380 (4)
N2—C7	1.372 (3)	C13—H13	0.9300
N2—C10	1.374 (3)	C14—C15	1.388 (3)
C1—C2	1.401 (3)	C14—H14	0.9300
C1—C10^{i}	1.410 (3)	C15—C16	1.383 (3)
C1—C16	1.500 (3)	C15—H15	0.9300
C2—C3	1.445 (3)	C17—C18	1.385 (3)
C3—C4	1.369 (3)	C17—C22	1.394 (3)
C3—C23	1.542 (3)	C18—C19	1.390 (3)
C4—C5	1.445 (3)	C18—H18	0.9300
C4—C24	1.533 (3)	C19—C20	1.380 (3)
C5—C6	1.400 (3)	C19—H19	0.9300
C6—C7	1.407 (3)	C20—C21	1.391 (3)
C6—C17	1.498 (3)	C20—H20	0.9300
C7—C8	1.451 (3)	C21—C22	1.378 (3)
C8—C9	1.347 (3)	C21—H21	0.9300
C8—H8	0.9300	C22—H22	0.9300
C9—C10	1.448 (3)	C23—H23A	0.9600
C9—H9	0.9300	C23—H23B	0.9600
C10—C1^{i}	1.410 (3)	C23—H23C	0.9600

C11—C12	1.387 (3)	C24—H24A	0.9600
C11—C16	1.387 (3)	C24—H24B	0.9600
C11—H11	0.9300	C24—H24C	0.9600
C5—N1—C2	110.38 (16)	C12—C13—H13	120.1
C5—N1—H1	124.8	C14—C13—H13	120.1
C2—N1—H1	124.8	C13—C14—C15	119.8 (2)
C7—N2—C10	105.35 (16)	C13—C14—H14	120.1
C2—C1—C10^{i}	125.76 (18)	C15—C14—H14	120.1
C2—C1—C16	118.59 (17)	C16—C15—C14	120.8 (2)
C10^{i}—C1—C16	115.34 (17)	C16—C15—H15	119.6
N1—C2—C1	123.78 (17)	C14—C15—H15	119.6
N1—C2—C3	106.97 (17)	C15—C16—C11	118.7 (2)
C1—C2—C3	129.22 (18)	C15—C16—C1	119.15 (19)
C4—C3—C2	107.69 (17)	C11—C16—C1	122.10 (19)
C4—C3—C23	124.25 (18)	C18—C17—C22	119.04 (19)
C2—C3—C23	128.01 (18)	C18—C17—C6	121.66 (18)
C3—C4—C5	107.95 (17)	C22—C17—C6	119.20 (18)
C3—C4—C24	124.69 (18)	C17—C18—C19	120.5 (2)
C5—C4—C24	127.12 (18)	C17—C18—H18	119.8
N1—C5—C6	124.65 (18)	C19—C18—H18	119.8
N1—C5—C4	106.94 (17)	C20—C19—C18	120.1 (2)
C6—C5—C4	128.40 (18)	C20—C19—H19	120.0
C5—C6—C7	126.31 (18)	C18—C19—H19	120.0
C5—C6—C17	118.39 (18)	C19—C20—C21	119.7 (2)
C7—C6—C17	115.09 (17)	C19—C20—H20	120.1
N2—C7—C6	128.03 (18)	C21—C20—H20	120.1
N2—C7—C8	110.49 (17)	C22—C21—C20	120.1 (2)
C6—C7—C8	121.43 (18)	C22—C21—H21	119.9
C9—C8—C7	106.77 (18)	C20—C21—H21	119.9
C9—C8—H8	126.6	C21—C22—C17	120.5 (2)
C7—C8—H8	126.6	C21—C22—H22	119.7
C8—C9—C10	106.79 (18)	C17—C22—H22	119.7
C8—C9—H9	126.6	C3—C23—H23A	109.5
C10—C9—H9	126.6	C3—C23—H23B	109.5
N2—C10—C1^{i}	127.27 (18)	H23A—C23—H23B	109.5
N2—C10—C9	110.60 (17)	C3—C23—H23C	109.5
C1^{i}—C10—C9	121.95 (18)	H23A—C23—H23C	109.5
C12—C11—C16	120.4 (2)	H23B—C23—H23C	109.5
C12—C11—H11	119.8	C4—C24—H24A	109.5
C16—C11—H11	119.8	C4—C24—H24B	109.5
C13—C12—C11	120.4 (2)	H24A—C24—H24B	109.5
C13—C12—H12	119.8	C4—C24—H24C	109.5
C11—C12—H12	119.8	H24A—C24—H24C	109.5
C12—C13—C14	119.9 (2)	H24B—C24—H24C	109.5

Symmetry codes: (i) $-x$, $-y+2$, $-z$.

Fig. 1

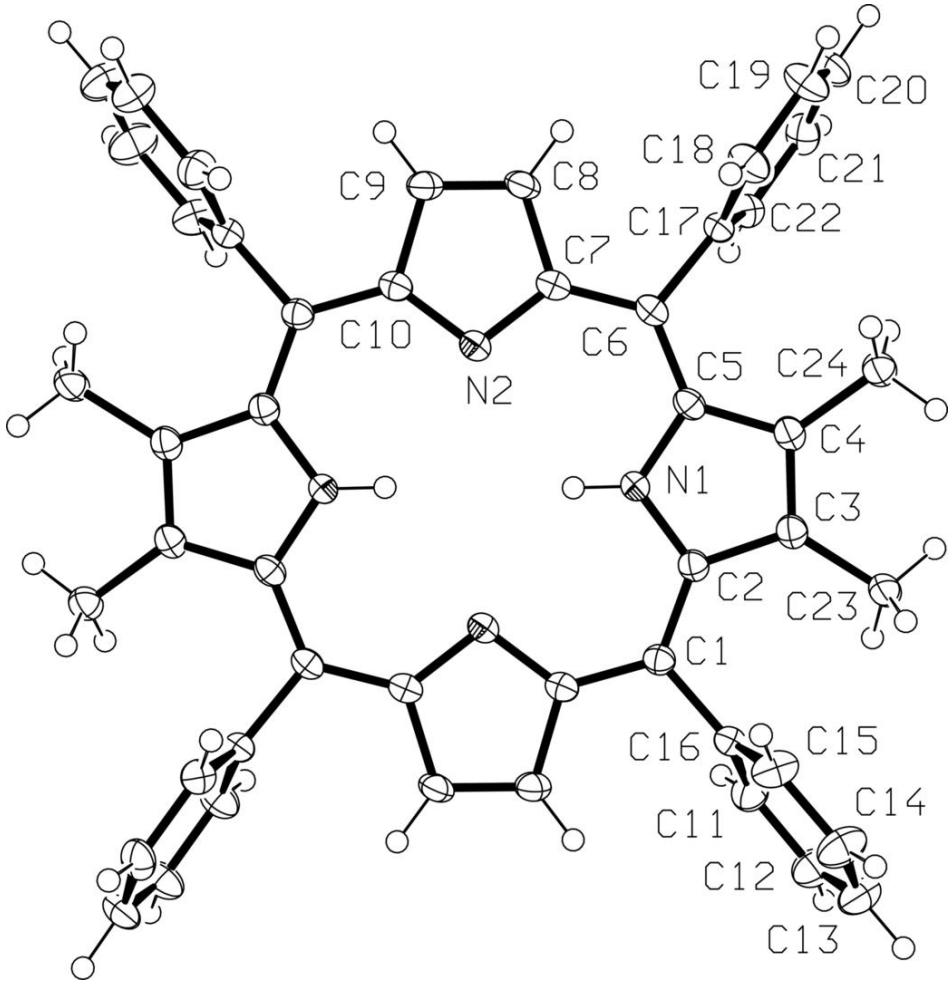
C19
C20
C18
C21
C9
C8
C17
C22
C7
C10
C6
C5
C24
N2
C4
N1
C3
C2
C23
C1
C16
C15
C14
C11
C12
C13

Fig. 2