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7-Nitro-5,10,15,20-tetraphenylporphyrin Dichloromethane Solvate

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Abstract

The title compound shows significant conformational distortion in the vicinity of the β-nitro group. This is attributed to steric interaction between a *meso*-phenyl and the β-nitro group. The overall degree of conformation distortion is moderate, the average deviation of the 24 macrocycle atoms from their least- squares plane being 0.08 Å. The largest displacements (0.33 Å from the plane of the four pyrrole nitrogen atoms) were found for the C_b-positions of the nitrated pyrrole ring.

Comment

The title compound was investigated with regard to potential steric interactions between the β-nitro group and the neighboring *meso*-phenyl substituent. The overall degree of macrocycle distortion is moderate, the average deviation of the 24 macrocycle atoms from their least-square plane being only 0.088 Å. Nevertheless, a more localized conformational influence of the nitro-group is observed. The average displacement of the C_b-carbons from the least-square plane of the four pyrrole nitrogen atoms (4 N-plane) is 0.17 Å. The respective average displacement values for the C_b carbons of individual pyrrole rings are: ring I (with nitro group) 0.33 Å, ring II 0.25 Å, ring III 0.03 Å, and ring IV 0.07 Å. The plane of the pyrrole rings are tilted against the 4 N-plane by 9° (ring I), 7.1° (ring II), 0.9° (ring III), and 3.0° (ring IV). Thus, the macrocycle shows definite distortions in the vicinity of the *meso*- phenyl/nitro-interaction which become progressively smaller which increasing distance from the β-nitro group. Displacements of the *meso*-carbons from the 4 N-plane are in the order of 0.02–0.04 Å. The nitro group is tilted against the 4 N-plane by 48.4°. There is no evidence for increased π-π-overlap between the nitro-group and the aromatic macrocycle.

The molecules form well separated layers with no evidence of π- stacking. The closest intermolecular contacts observed were N21—Cl2S (3.15 Å) and O1—H202 (2.51 Å). Related structures are a planar high-spin Ni(II) complex of 2,3,7,8,12,13,17-heptanitro-5,10,15,20- tetrakis(2,6-dichlorophenyl)porphyrin (Ozette *et al.*, 1997) and a saddle-distorted 7,12-dinitro-5,10,15,20-tetraphenylporphyrin (Dahal *et al.*, 1994). β-Nitroporphyrins have recently been shown to be excellent precursors for the preparation of fused pyrrolo- porphyrins (Jaquinod *et al.*, 1996).

Experimental

The compound was prepared synthetically as described by Giraudeau, A. *et al.* (1979). Crystals were grown from CH_2Cl_2/n-hexane and mounted according to Hope (1994).

Computing details

Data collection: Siemens P3; cell refinement: Siemens P3; data reduction: *XDISK*, *SHELXTL-Plus* (Sheldrick, 1994); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL93* (Sheldrick,

1993); molecular graphics: *XP*, *SHELXTL-Plus* (Sheldrick, 1994); software used to prepare material for publication: *SHELXL*, *SHELXTL-Plus* (Sheldrick, 1994).

7-Nitro-5,10,15,20-tetraphenylporphyrin

Crystal data

$C_{44}H_{29}N_5O_2 \cdot C_1H_2Cl_2$	$\gamma = 77.88\ (4)^\circ$
$M_r = 744.65$	$V = 1822.5\ (15)\ Å^3$
Triclinic, $P\overline{1}$	$Z = 2$
$a = 10.904\ (6)$ Å	Mo $K\alpha$
$b = 13.404\ (6)$ Å	$\mu = 0.23\ mm^{-1}$
$c = 13.683\ (6)$ Å	$T = 126\ (2)$ K
$\alpha = 88.97\ (4)^\circ$	0.7 × 0.2 × 0.2 mm
$\beta = 69.05\ (4)^\circ$	

Data collection

Siemens R3m/V diffractometer	4988 reflections with $I > 2\sigma(I)$
Absorption correction: empirical (using intensity measurements) Parkin et al. (1995)	$R_{int} = 0.036$
$T_{min} = 0.85$, $T_{max} = 0.96$	2 standard reflections
6821 measured reflections	every 198 reflections
6447 independent reflections	intensity decay: <1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$	487 parameters
$wR(F^2) = 0.153$	H-atom parameters constrained
$S = 1.04$	$\Delta\rho_{max} = 0.60\ e\ Å^{-3}$
6447 reflections	$\Delta\rho_{min} = -0.80\ e\ Å^{-3}$

Table 1
Selected geometric parameters (Å, °)

N21—C1	1.366 (4)	C7—C8	1.355 (5)
N21—C4	1.375 (4)	C8—C9	1.426 (4)
N22—C9	1.373 (4)	C9—C10	1.411 (4)
N22—C6	1.381 (4)	C10—C11	1.400 (4)
N23—C14	1.373 (4)	C11—C12	1.457 (4)
N23—C11	1.375 (4)	C12—C13	1.345 (4)
N24—C16	1.372 (4)	C13—C14	1.451 (4)
N24—C19	1.382 (4)	C14—C15	1.405 (4)
C1—C20	1.417 (4)	C15—C16	1.394 (4)
C1—C2	1.459 (4)	C16—C17	1.428 (4)

C2—C3	1.348 (4)	C17—C18	1.357 (4)
C2—N1	1.450 (4)	C18—C19	1.433 (4)
C3—C4	1.439 (4)	C19—C20	1.399 (4)
C4—C5	1.408 (4)	N1—O1	1.226 (3)
C5—C6	1.393 (4)	N1—O2	1.241 (3)
C6—C7	1.428 (4)		
C1—N21—C4	106.6 (2)	C11—C10—C9	124.4 (3)
C9—N22—C6	110.3 (2)	N23—C11—C10	126.0 (3)
C14—N23—C11	105.0 (2)	N23—C11—C12	110.6 (3)
C16—N24—C19	110.6 (2)	C10—C11—C12	123.4 (3)
N21—C1—C20	125.9 (3)	C13—C12—C11	106.7 (3)
N21—C1—C2	108.5 (2)	C12—C13—C14	106.6 (3)
C20—C1—C2	125.6 (3)	N23—C14—C15	126.1 (3)
C3—C2—N1	121.2 (3)	N23—C14—C13	111.0 (3)
C3—C2—C1	108.4 (3)	C15—C14—C13	122.8 (3)
N1—C2—C1	130.0 (2)	C16—C15—C14	125.7 (3)
C2—C3—C4	105.7 (3)	N24—C16—C15	126.7 (3)
N21—C4—C5	126.3 (3)	N24—C16—C17	106.5 (2)
N21—C4—C3	110.8 (2)	C15—C16—C17	126.9 (3)
C5—C4—C3	122.9 (3)	C18—C17—C16	108.5 (3)
C6—C5—C4	125.8 (3)	C17—C18—C19	108.4 (3)
N22—C6—C5	126.6 (3)	N24—C19—C20	126.6 (3)
N22—C6—C7	106.0 (3)	N24—C19—C18	106.0 (2)
C5—C6—C7	127.4 (3)	C20—C19—C18	127.3 (3)
C8—C7—C6	108.7 (3)	C19—C20—C1	124.3 (3)
C7—C8—C9	108.3 (3)	O1—N1—O2	123.7 (3)
N22—C9—C10	126.5 (3)	O1—N1—C2	118.8 (2)
N22—C9—C8	106.6 (3)	O2—N1—C2	117.4 (2)
C10—C9—C8	126.9 (3)		

Acknowledgements

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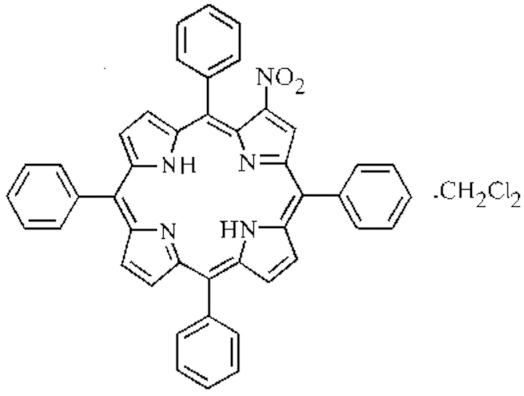
Scheme 1



supplementary materials

7-Nitro-5,10,15,20-tetraphenylporphyrin

Crystal data

$C_{44}H_{29}N_5O_2 \cdot C_1H_2Cl_2$	$F_{000} = 772$
$M_r = 744.65$	$D_x = 1.357$ Mg m^{-3}
Triclinic, $P\overline{1}$	Melting point: n/d K
$a = 10.904$ (6) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 13.404$ (6) Å	Cell parameters from 35 reflections
$c = 13.683$ (6) Å	$\theta = 22$–25º
$\alpha = 88.97$ (4)º	$\mu = 0.23$ mm^{-1}
$\beta = 69.05$ (4)º	$T = 126$ (2) K
$\gamma = 77.88$ (4)º	Parallelepiped, red
$V = 1822.5$ (15) Å^3	0.7 × 0.2 × 0.2 mm
$Z = 2$	

Data collection

Siemens R3m/V diffractometer	$R_{int} = 0.036$
Radiation source: normal-focus sealed tube	$\theta_{max} = 25.1$º
Monochromator: graphite	$\theta_{min} = 1.6$º
$T = 126(2)$ K	$h = -11 \rightarrow 12$
ω–scans	$k = -15 \rightarrow 15$
Absorption correction: empirical (using intensity measurements) Parkin et al. (1995)	$l = 0 \rightarrow 16$
$T_{min} = 0.85$, $T_{max} = 0.96$	2 standard reflections
6821 measured reflections	every 198 reflections
6447 independent reflections	intensity decay: <1%
4988 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: calc
$R[F^2 > 2\sigma(F^2)] = 0.060$	H-atom parameters constrained
$wR(F^2) = 0.153$	Calculated $w = 1/[\sigma^2(F_o^2) + (0.0649P)^2 + 1.7996P]$ where $P = (F_o^2 + 2F_c^2)/3$?
$S = 1.04$	$\Delta\rho_{max} = 0.60$ e Å^{-3}
6447 reflections	$\Delta\rho_{min} = -0.80$ e Å^{-3}
487 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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. Hydrogen atoms were placed in calculated positions and refined using a riding model. The β- and pyrrole hydrogen atoms were initially located in difference maps. An absorption correction was performed using the program *XABS2* (Parkin, Moezzi & Hope, 1995). All calculations were performed using the *SHELXTL-Plus* program system (Sheldrick, 1994).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N21	−0.3788 (2)	0.6208 (2)	0.8117 (2)	0.0273 (5)
N22	−0.4756 (2)	0.7199 (2)	1.0248 (2)	0.0320 (6)
H22	−0.4956 (2)	0.7326 (2)	0.9683 (2)	0.038*
N23	−0.6259 (2)	0.8905 (2)	0.9534 (2)	0.0295 (5)
N24	−0.5330 (2)	0.7926 (2)	0.7418 (2)	0.0275 (5)
H24	−0.5232 (2)	0.7754 (2)	0.8014 (2)	0.033*
C1	−0.3529 (3)	0.5820 (2)	0.7130 (2)	0.0256 (6)
C2	−0.2817 (3)	0.4754 (2)	0.7026 (2)	0.0276 (6)
C3	−0.2625 (3)	0.4522 (2)	0.7930 (2)	0.0304 (6)
H3	−0.2182 (3)	0.3886 (2)	0.8087 (2)	0.037*
C4	−0.3230 (3)	0.5440 (2)	0.8609 (2)	0.0280 (6)
C5	−0.3196 (3)	0.5515 (2)	0.9623 (2)	0.0300 (6)
C51	−0.2332 (3)	0.4645 (2)	0.9944 (2)	0.0286 (6)
C52	−0.0952 (3)	0.4392 (2)	0.9391 (2)	0.0360 (7)
H52	−0.0562 (3)	0.4766 (2)	0.8808 (2)	0.043*
C53	−0.0135 (3)	0.3594 (3)	0.9687 (3)	0.0420 (8)
H53	0.0807 (3)	0.3425 (3)	0.9302 (3)	0.050*
C54	−0.0690 (3)	0.3046 (2)	1.0537 (3)	0.0405 (8)
H54	−0.0131 (3)	0.2507 (2)	1.0742 (3)	0.049*
C55	−0.2059 (3)	0.3287 (3)	1.1086 (3)	0.0413 (8)
H55	−0.2443 (3)	0.2908 (3)	1.1666 (3)	0.050*
C56	−0.2882 (3)	0.4081 (2)	1.0796 (2)	0.0366 (7)
H56	−0.3824 (3)	0.4240 (2)	1.1180 (2)	0.044*
C6	−0.3877 (3)	0.6338 (2)	1.0357 (2)	0.0318 (7)
C7	−0.3825 (3)	0.6460 (2)	1.1375 (2)	0.0370 (7)
H7	−0.3282 (3)	0.5997 (2)	1.1668 (2)	0.044*
C8	−0.4678 (3)	0.7346 (3)	1.1855 (2)	0.0401 (8)
H8	−0.4849 (3)	0.7603 (3)	1.2545 (2)	0.048*
C9	−0.5276 (3)	0.7829 (2)	1.1147 (2)	0.0319 (7)
C10	−0.6184 (3)	0.8785 (2)	1.1317 (2)	0.0316 (7)
C101	−0.6745 (3)	0.9271 (2)	1.2407 (2)	0.0321 (7)
C102	−0.7514 (3)	0.8766 (3)	1.3225 (2)	0.0406 (8)
H102	−0.7646 (3)	0.8113 (3)	1.3083 (2)	0.049*
C103	−0.8084 (4)	0.9205 (3)	1.4236 (3)	0.0469 (9)

H103	−0.8612 (4)	0.8856 (3)	1.4783 (3)	0.056*
C104	−0.7889 (3)	1.0151 (3)	1.4456 (3)	0.0441 (8)
H104	−0.8277 (3)	1.0450 (3)	1.5152 (3)	0.053*
C105	−0.7123 (3)	1.0659 (3)	1.3654 (3)	0.0399 (8)
H105	−0.6989 (3)	1.1310 (3)	1.3801 (3)	0.048*
C106	−0.6554 (3)	1.0223 (2)	1.2638 (2)	0.0344 (7)
H106	−0.6028 (3)	1.0576 (2)	1.2094 (2)	0.041*
C11	−0.6608 (3)	0.9282 (2)	1.0547 (2)	0.0302 (6)
C12	−0.7510 (3)	1.0286 (2)	1.0732 (2)	0.0367 (7)
H12	−0.7896 (3)	1.0700 (2)	1.1369 (2)	0.044*
C13	−0.7692 (3)	1.0514 (2)	0.9825 (2)	0.0367 (7)
H13	−0.8219 (3)	1.1125 (2)	0.9694 (2)	0.044*
C14	−0.6926 (3)	0.9646 (2)	0.9085 (2)	0.0303 (6)
C15	−0.6893 (3)	0.9604 (2)	0.8050 (2)	0.0292 (6)
C151	−0.7725 (3)	1.0489 (2)	0.7728 (2)	0.0289 (6)
C152	−0.9126 (3)	1.0675 (2)	0.8167 (2)	0.0340 (7)
H152	−0.9548 (3)	1.0235 (2)	0.8667 (2)	0.041*
C153	−0.9909 (3)	1.1501 (3)	0.7877 (3)	0.0416 (8)
H153	−1.0863 (3)	1.1623 (3)	0.8181 (3)	0.050*
C154	−0.9302 (3)	1.2142 (3)	0.7150 (3)	0.0414 (8)
H154	−0.9837 (3)	1.2701 (3)	0.6948 (3)	0.050*
C155	−0.7917 (3)	1.1971 (3)	0.6716 (3)	0.0423 (8)
H155	−0.7501 (3)	1.2418 (3)	0.6222 (3)	0.051*
C156	−0.7129 (3)	1.1150 (2)	0.6997 (2)	0.0366 (7)
H156	−0.6176 (3)	1.1035 (2)	0.6690 (2)	0.044*
C16	−0.6131 (3)	0.8816 (2)	0.7288 (2)	0.0290 (6)
C17	−0.6017 (3)	0.8780 (2)	0.6216 (2)	0.0316 (7)
H17	−0.6479 (3)	0.9285 (2)	0.5899 (2)	0.038*
C18	−0.5137 (3)	0.7905 (2)	0.5726 (2)	0.0310 (7)
H18	−0.4858 (3)	0.7703 (2)	0.5004 (2)	0.037*
C19	−0.4699 (3)	0.7337 (2)	0.6484 (2)	0.0279 (6)
C20	−0.3839 (3)	0.6372 (2)	0.6324 (2)	0.0266 (6)
C201	−0.3151 (3)	0.5930 (2)	0.5222 (2)	0.0255 (6)
C202	−0.3890 (3)	0.5730 (2)	0.4621 (2)	0.0294 (6)
H202	−0.4845 (3)	0.5903 (2)	0.4907 (2)	0.035*
C203	−0.3237 (3)	0.5285 (2)	0.3617 (2)	0.0347 (7)
H203	−0.3743 (3)	0.5139 (2)	0.3220 (2)	0.042*
C204	−0.1835 (3)	0.5047 (2)	0.3184 (2)	0.0364 (7)
H204	−0.1386 (3)	0.4729 (2)	0.2498 (2)	0.044*
C205	−0.1100 (3)	0.5276 (2)	0.3757 (2)	0.0334 (7)
H205	−0.0146 (3)	0.5137 (2)	0.3452 (2)	0.040*
C206	−0.1748 (3)	0.5707 (2)	0.4772 (2)	0.0279 (6)
H206	−0.1235 (3)	0.5852 (2)	0.5164 (2)	0.033*
N1	−0.2484 (3)	0.3972 (2)	0.6198 (2)	0.0334 (6)
O1	−0.3360 (2)	0.3861 (2)	0.5871 (2)	0.0425 (6)
O2	−0.1330 (2)	0.3427 (2)	0.5888 (2)	0.0426 (6)
C1S	−0.0197 (4)	0.2456 (3)	0.3472 (3)	0.0638 (12)
H1S1	−0.0005 (4)	0.2236 (3)	0.4107 (3)	0.077*
H1S2	−0.0986 (4)	0.3037 (3)	0.3689 (3)	0.077*

Cl1S	−0.05989 (11)	0.14540 (9)	0.29498 (7)	0.0651 (3)
Cl2S	0.11905 (9)	0.28716 (7)	0.25975 (8)	0.0531 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N21	0.0246 (12)	0.0304 (13)	0.0267 (12)	−0.0041 (10)	−0.0101 (10)	0.0032 (10)
N22	0.0352 (14)	0.0340 (14)	0.0259 (13)	0.0012 (11)	−0.0150 (11)	0.0014 (11)
N23	0.0307 (13)	0.0291 (13)	0.0272 (12)	−0.0010 (10)	−0.0117 (10)	0.0016 (10)
N24	0.0299 (13)	0.0282 (13)	0.0245 (12)	−0.0022 (10)	−0.0125 (10)	0.0025 (10)
C1	0.0223 (14)	0.0272 (15)	0.0278 (14)	−0.0055 (12)	−0.0098 (12)	0.0029 (12)
C2	0.0262 (15)	0.0270 (15)	0.0293 (15)	−0.0046 (12)	−0.0105 (12)	−0.0007 (12)
C3	0.030 (2)	0.028 (2)	0.034 (2)	−0.0053 (12)	−0.0133 (13)	0.0053 (12)
C4	0.0259 (15)	0.029 (2)	0.0295 (15)	−0.0054 (12)	−0.0109 (12)	0.0034 (12)
C5	0.028 (2)	0.032 (2)	0.030 (2)	−0.0053 (13)	−0.0116 (12)	0.0057 (12)
C51	0.031 (2)	0.030 (2)	0.0278 (15)	−0.0032 (12)	−0.0148 (12)	0.0017 (12)
C52	0.030 (2)	0.043 (2)	0.034 (2)	−0.0066 (14)	−0.0105 (13)	0.0067 (14)
C53	0.028 (2)	0.046 (2)	0.046 (2)	0.0051 (14)	−0.0127 (14)	−0.002 (2)
C54	0.045 (2)	0.033 (2)	0.044 (2)	0.0041 (15)	−0.024 (2)	0.0040 (14)
C55	0.045 (2)	0.039 (2)	0.043 (2)	−0.010 (2)	−0.019 (2)	0.0151 (15)
C56	0.033 (2)	0.039 (2)	0.039 (2)	−0.0067 (14)	−0.0149 (14)	0.0089 (14)
C6	0.030 (2)	0.035 (2)	0.029 (2)	−0.0003 (13)	−0.0128 (13)	0.0019 (13)
C7	0.041 (2)	0.039 (2)	0.032 (2)	0.0019 (14)	−0.0186 (14)	0.0034 (14)
C8	0.045 (2)	0.045 (2)	0.030 (2)	0.000 (2)	−0.0175 (15)	−0.0013 (14)
C9	0.034 (2)	0.034 (2)	0.0264 (15)	−0.0018 (13)	−0.0138 (13)	0.0014 (12)
C10	0.032 (2)	0.032 (2)	0.031 (2)	−0.0053 (13)	−0.0125 (13)	0.0016 (13)
C101	0.029 (2)	0.038 (2)	0.028 (2)	−0.0017 (13)	−0.0114 (13)	0.0004 (13)
C102	0.050 (2)	0.036 (2)	0.034 (2)	−0.008 (2)	−0.0128 (15)	0.0014 (14)
C103	0.059 (2)	0.050 (2)	0.028 (2)	−0.013 (2)	−0.012 (2)	0.0078 (15)
C104	0.043 (2)	0.056 (2)	0.030 (2)	−0.001 (2)	−0.0142 (15)	−0.004 (2)
C105	0.038 (2)	0.041 (2)	0.044 (2)	−0.0073 (15)	−0.0189 (15)	−0.0061 (15)
C106	0.030 (2)	0.041 (2)	0.032 (2)	−0.0078 (14)	−0.0114 (13)	0.0032 (13)
C11	0.0273 (15)	0.032 (2)	0.0280 (15)	−0.0005 (12)	−0.0093 (12)	−0.0008 (12)
C12	0.036 (2)	0.036 (2)	0.033 (2)	0.0050 (14)	−0.0129 (14)	−0.0055 (13)
C13	0.037 (2)	0.032 (2)	0.036 (2)	0.0074 (14)	−0.0151 (14)	−0.0043 (13)
C14	0.0271 (15)	0.031 (2)	0.032 (2)	−0.0014 (12)	−0.0116 (12)	0.0022 (12)
C15	0.0270 (15)	0.029 (2)	0.0301 (15)	−0.0031 (12)	−0.0105 (12)	0.0027 (12)
C151	0.033 (2)	0.0261 (15)	0.0286 (15)	−0.0011 (12)	−0.0150 (13)	−0.0003 (12)
C152	0.033 (2)	0.033 (2)	0.038 (2)	−0.0059 (13)	−0.0156 (14)	0.0051 (13)
C153	0.031 (2)	0.041 (2)	0.052 (2)	−0.0005 (14)	−0.018 (2)	0.002 (2)
C154	0.046 (2)	0.034 (2)	0.045 (2)	0.0027 (15)	−0.024 (2)	0.0038 (15)
C155	0.047 (2)	0.036 (2)	0.044 (2)	−0.005 (2)	−0.018 (2)	0.0130 (15)
C156	0.030 (2)	0.036 (2)	0.041 (2)	−0.0033 (13)	−0.0122 (14)	0.0059 (14)
C16	0.0279 (15)	0.030 (2)	0.0301 (15)	−0.0043 (12)	−0.0136 (12)	0.0053 (12)
C17	0.032 (2)	0.032 (2)	0.031 (2)	−0.0012 (13)	−0.0153 (13)	0.0045 (13)
C18	0.035 (2)	0.034 (2)	0.0263 (15)	−0.0036 (13)	−0.0154 (13)	0.0039 (12)
C19	0.0280 (15)	0.028 (2)	0.0298 (15)	−0.0059 (12)	−0.0129 (12)	0.0030 (12)
C20	0.0261 (14)	0.028 (2)	0.0279 (14)	−0.0085 (12)	−0.0115 (12)	0.0028 (12)

C201	0.0293 (15)	0.0229 (14)	0.0253 (14)	−0.0044 (12)	−0.0120 (12)	0.0057 (11)
C202	0.031 (2)	0.028 (2)	0.032 (2)	−0.0069 (12)	−0.0148 (13)	0.0055 (12)
C203	0.043 (2)	0.037 (2)	0.031 (2)	−0.0123 (14)	−0.0202 (14)	0.0050 (13)
C204	0.043 (2)	0.036 (2)	0.027 (2)	−0.0098 (14)	−0.0091 (14)	−0.0008 (13)
C205	0.028 (2)	0.033 (2)	0.035 (2)	−0.0045 (13)	−0.0068 (13)	0.0022 (13)
C206	0.0282 (15)	0.0259 (15)	0.032 (2)	−0.0055 (12)	−0.0146 (12)	0.0059 (12)
N1	0.0390 (15)	0.0289 (14)	0.0380 (14)	−0.0050 (12)	−0.0223 (12)	0.0071 (11)
O1	0.0496 (14)	0.0383 (13)	0.0526 (14)	−0.0119 (11)	−0.0329 (12)	0.0051 (10)
O2	0.0422 (13)	0.0352 (13)	0.0467 (13)	0.0077 (10)	−0.0204 (11)	−0.0059 (10)
C1S	0.067 (3)	0.055 (2)	0.053 (2)	−0.025 (2)	0.004 (2)	−0.009 (2)
Cl1S	0.0702 (7)	0.0852 (8)	0.0459 (5)	−0.0450 (6)	−0.0119 (5)	−0.0019 (5)
Cl2S	0.0466 (5)	0.0408 (5)	0.0662 (6)	−0.0150 (4)	−0.0104 (4)	0.0024 (4)

Geometric parameters (Å, °)

N21—C1	1.366 (4)	C103—C104	1.385 (5)
N21—C4	1.375 (4)	C104—C105	1.387 (5)
N22—C9	1.373 (4)	C105—C106	1.385 (4)
N22—C6	1.381 (4)	C11—C12	1.457 (4)
N23—C14	1.373 (4)	C12—C13	1.345 (4)
N23—C11	1.375 (4)	C13—C14	1.451 (4)
N24—C16	1.372 (4)	C14—C15	1.405 (4)
N24—C19	1.382 (4)	C15—C16	1.394 (4)
C1—C20	1.417 (4)	C15—C151	1.498 (4)
C1—C2	1.459 (4)	C151—C152	1.394 (4)
C2—C3	1.348 (4)	C151—C156	1.397 (4)
C2—N1	1.450 (4)	C152—C153	1.394 (4)
C3—C4	1.439 (4)	C153—C154	1.381 (5)
C4—C5	1.408 (4)	C154—C155	1.380 (5)
C5—C6	1.393 (4)	C155—C156	1.386 (4)
C5—C51	1.503 (4)	C16—C17	1.428 (4)
C51—C52	1.390 (4)	C17—C18	1.357 (4)
C51—C56	1.396 (4)	C18—C19	1.433 (4)
C52—C53	1.394 (4)	C19—C20	1.399 (4)
C53—C54	1.382 (5)	C20—C201	1.492 (4)
C54—C55	1.379 (5)	C201—C206	1.397 (4)
C55—C56	1.390 (4)	C201—C202	1.404 (4)
C6—C7	1.428 (4)	C202—C203	1.379 (4)
C7—C8	1.355 (5)	C203—C204	1.394 (5)
C8—C9	1.426 (4)	C204—C205	1.382 (4)
C9—C10	1.411 (4)	C205—C206	1.385 (4)
C10—C11	1.400 (4)	N1—O1	1.226 (3)
C10—C101	1.495 (4)	N1—O2	1.241 (3)
C101—C106	1.395 (4)	C1S—Cl1S	1.735 (4)
C101—C102	1.398 (4)	C1S—Cl2S	1.751 (4)
C102—C103	1.381 (5)		
C1—N21—C4	106.6 (2)	C105—C106—C101	120.6 (3)
C9—N22—C6	110.3 (2)	N23—C11—C10	126.0 (3)
C14—N23—C11	105.0 (2)	N23—C11—C12	110.6 (3)

C16—N24—C19	110.6 (2)	C10—C11—C12	123.4 (3)
N21—C1—C20	125.9 (3)	C13—C12—C11	106.7 (3)
N21—C1—C2	108.5 (2)	C12—C13—C14	106.6 (3)
C20—C1—C2	125.6 (3)	N23—C14—C15	126.1 (3)
C3—C2—N1	121.2 (3)	N23—C14—C13	111.0 (3)
C3—C2—C1	108.4 (3)	C15—C14—C13	122.8 (3)
N1—C2—C1	130.0 (2)	C16—C15—C14	125.7 (3)
C2—C3—C4	105.7 (3)	C16—C15—C151	116.9 (2)
N21—C4—C5	126.3 (3)	C14—C15—C151	117.4 (2)
N21—C4—C3	110.8 (2)	C152—C151—C156	118.6 (3)
C5—C4—C3	122.9 (3)	C152—C151—C15	120.0 (3)
C6—C5—C4	125.8 (3)	C156—C151—C15	121.4 (3)
C6—C5—C51	116.5 (3)	C153—C152—C151	120.5 (3)
C4—C5—C51	117.7 (3)	C154—C153—C152	120.1 (3)
C52—C51—C56	118.7 (3)	C155—C154—C153	119.9 (3)
C52—C51—C5	119.9 (3)	C154—C155—C156	120.4 (3)
C56—C51—C5	121.4 (3)	C155—C156—C151	120.5 (3)
C51—C52—C53	120.5 (3)	N24—C16—C15	126.7 (3)
C54—C53—C52	120.2 (3)	N24—C16—C17	106.5 (2)
C55—C54—C53	119.6 (3)	C15—C16—C17	126.9 (3)
C54—C55—C56	120.5 (3)	C18—C17—C16	108.5 (3)
C55—C56—C51	120.4 (3)	C17—C18—C19	108.4 (3)
N22—C6—C5	126.6 (3)	N24—C19—C20	126.6 (3)
N22—C6—C7	106.0 (3)	N24—C19—C18	106.0 (2)
C5—C6—C7	127.4 (3)	C20—C19—C18	127.3 (3)
C8—C7—C6	108.7 (3)	C19—C20—C1	124.3 (3)
C7—C8—C9	108.3 (3)	C19—C20—C201	117.2 (2)
N22—C9—C10	126.5 (3)	C1—C20—C201	118.5 (2)
N22—C9—C8	106.6 (3)	C206—C201—C202	118.9 (3)
C10—C9—C8	126.9 (3)	C206—C201—C20	120.0 (2)
C11—C10—C9	124.4 (3)	C202—C201—C20	121.2 (2)
C11—C10—C101	118.9 (3)	C203—C202—C201	120.4 (3)
C9—C10—C101	116.7 (3)	C202—C203—C204	120.2 (3)
C106—C101—C102	118.4 (3)	C205—C204—C203	119.8 (3)
C106—C101—C10	122.5 (3)	C204—C205—C206	120.4 (3)
C102—C101—C10	119.1 (3)	C205—C206—C201	120.3 (3)
C103—C102—C101	120.8 (3)	O1—N1—O2	123.7 (3)
C102—C103—C104	120.2 (3)	O1—N1—C2	118.8 (2)
C103—C104—C105	119.7 (3)	O2—N1—C2	117.4 (2)
C104—C105—C106	120.2 (3)	Cl1S—C1S—Cl2S	113.5 (2)