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Oxomemazine hydrochloride

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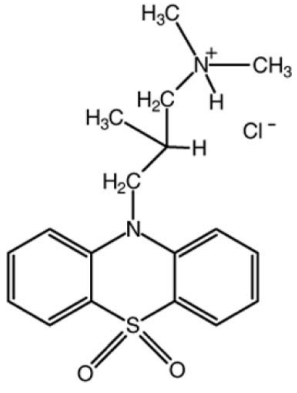
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.079; wR factor = 0.229; data-to-parameter ratio = 16.3.

In the title compound [systematic name: 3-(5,5-dioxophenothiazin-10-yl)-*N*,*N*,2-trimethylpropanaminium chloride], $C_{18}H_{23}N_2O_2S^+\cdot Cl^-$, the dihedral angle between the two outer aromatic rings of the phenothiazine unit is 30.5 (2)°. In the crystal, the components are linked by N—H···Cl and C—H···Cl hydrogen bonds and C—H···π interactions.

Related literature

For background to oxomemazine, see: Amin *et al.* (2008); El-Didamony, (2005). For related structures, see: Harrison *et al.* (2007); Jasinski *et al.* (2011).



Experimental

Crystal data

$C_{18}H_{23}N_2O_2S^+\cdot Cl^-$
M_r = 366.90
Triclinic, $P\overline{1}$
a = 7.6364 (7) Å
b = 10.4177 (9) Å
c = 12.4732 (10) Å
α = 103.478 (7)°
β = 90.624 (7)°
γ = 109.852 (8)°
V = 903.21 (15) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 3.06 mm^{-1}
T = 295 K
0.32 × 0.25 × 0.24 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Absorption correction: refined from ΔF [*XABS2* (Parkin *et al.*, 1995) in *WinGX* (Farrugia (1999)]
T_{min} = 0.441, T_{max} = 0.528
6466 measured reflections
3598 independent reflections
3120 reflections with $I > 2\sigma(I)$
R_{int} = 0.0422

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.229
S = 1.09
3598 reflections
221 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*2 is the centroid of the C1–C6 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*B*···Cl1	0.91	2.18	3.027 (4)	155
C13—H13*A*···Cl1^{i}	0.97	2.80	3.608 (4)	141
C13—H13*B*···Cl1	0.97	2.76	3.692 (4)	161
C17—H17*B*···*Cg*2^{ii}	0.96	2.62	3.559 (6)	166

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5925).

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supporting information

Acta Cryst. (2011). E**67**, o1875 [doi:10.1107/S1600536811025372]

Oxomemazine hydrochloride

M. S. Siddegowda, Ray J. Butcher, Mehmet Akkurt, H. S. Yathirajan and A. R. Ramesh

S1. Comment

Oxomemazine is an antihistamine and anticholinergic of the phenothiazine chemical class used for the treatment of cough. The extractive spectrophotometric methods for the determination of oxomemazine hydrochloride in bulk and pharmaceutical formulations using some organic dyes is described (El-Didamony, 2005; Amin *et al.*, 2008). The crystal structures of dioxopromethazinium picrate (Harrison *et al.*, 2007) and 1-(10*H*-phenothiazin-2-yl)ethanone (Jasinski *et al.*, 2011) have been reported. We now report the crystal structure of the title compound, (I).

In the molecule of (I), (Fig. 1), the dihedral angle between the two aromatic rings of the phenothiazine unit is 30.5 (2)°. All bond lengths and angles in (I) are normal. In the crystal structure, N—H···Cl, C—H···Cl hydrogen bonds (Table 1, Fig. 2) and C—H···π interactions help to establish the packing of (I).

S2. Experimental

The title compound was obtained as a gift sample from *R. L*. Fine Chem., Bangalore, India. X-ray quality crystals were obtained from a 1:1 mixture of dimethylformamide and ethanol by slow evaporation (m.p.: 520–523 K).

S3. Refinement

All H atoms were located geometrically (methyl C—H = 0.98 Å, methylene C—H = 0.99 Å, aromatic C—H = 0.95Å and N—H = 0.91 Å) and refined using a riding model. Their isotropic displacement parameters were set to 1.2 (or 1.5 for the methyl group) times the U_{eq} of the parent atom. 23 poorly fitted reflections were omitted from the refinement.

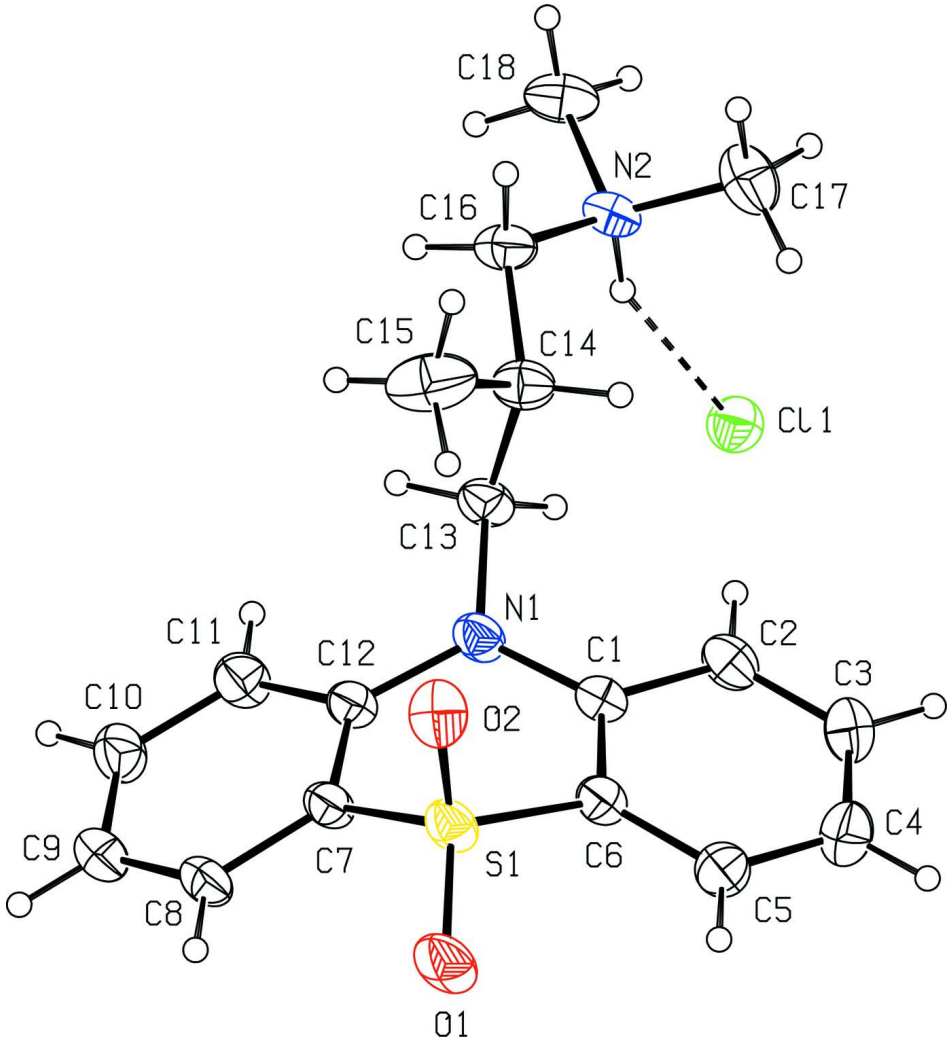

Figure 1

View of (I) showing displacement ellipsoids for non-H atoms drawn at the 30% probability level.

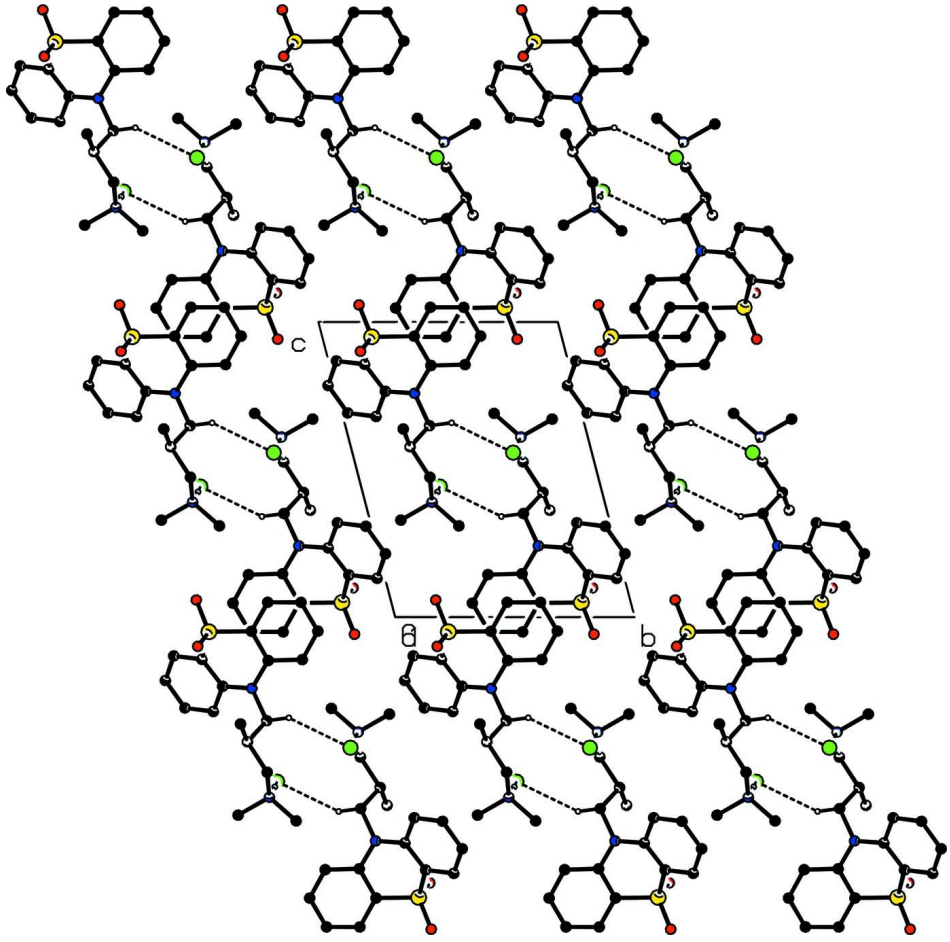

Figure 2

A view of the crystal packing and hydrogen bonding of (I) shown down the *a* axis.

3-(5,5-dioxophenothiazin-10-yl)-*N*,*N*,2-trimethylpropanaminium chloride

Crystal data

$C_{18}H_{23}N_2O_2S^+\cdot Cl^-$
$M_r = 366.90$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.6364\ (7)$ Å
$b = 10.4177\ (9)$ Å
$c = 12.4732\ (10)$ Å
$\alpha = 103.478\ (7)°$
$\beta = 90.624\ (7)°$
$\gamma = 109.852\ (8)°$
$V = 903.21\ (15)$ Å^3
$Z = 2$
$F(000) = 388$
$D_x = 1.349$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 3224 reflections
$\theta = 4.7–75.0°$
$\mu = 3.06$ mm^{-1}
$T = 295$ K
Prism, colourless
0.32 × 0.25 × 0.24 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm^{-1}
ω scans
Absorption correction: part of the refinement model (ΔF)
[*XABS2* (Parkin *et al.*, 1995) in the *WinGX* (Farrugia (1999).

T_{min} = 0.441, T_{max} = 0.528
6466 measured reflections
3598 independent reflections
3120 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

θ_{max} = 75.8°, θ_{min} = 4.7°
h = −9→9
k = −12→12
l = 0→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.229
S = 1.09
3598 reflections
221 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1168P)^2 + 1.2778P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.59166 (14)	0.20629 (10)	0.95014 (7)	0.0449 (3)
O1	0.5426 (5)	0.1883 (4)	1.0580 (2)	0.0663 (10)
O2	0.7225 (4)	0.1441 (3)	0.9009 (3)	0.0587 (10)
N1	0.5526 (5)	0.3244 (3)	0.7585 (3)	0.0434 (9)
N2	0.5857 (5)	0.2792 (4)	0.3894 (3)	0.0448 (10)
C1	0.4037 (5)	0.2045 (4)	0.7654 (3)	0.0401 (10)
C2	0.2542 (6)	0.1382 (4)	0.6801 (3)	0.0492 (11)
C3	0.1031 (6)	0.0237 (5)	0.6921 (4)	0.0552 (14)
C4	0.0937 (6)	−0.0284 (5)	0.7851 (4)	0.0590 (14)
C5	0.2388 (6)	0.0333 (4)	0.8684 (4)	0.0511 (12)
C6	0.3941 (5)	0.1471 (4)	0.8570 (3)	0.0412 (10)
C7	0.6735 (5)	0.3847 (4)	0.9521 (3)	0.0412 (11)
C8	0.7662 (6)	0.4839 (4)	1.0502 (3)	0.0495 (11)
C9	0.8514 (6)	0.6230 (5)	1.0501 (4)	0.0547 (12)
C10	0.8428 (6)	0.6621 (4)	0.9525 (4)	0.0540 (11)
C11	0.7472 (6)	0.5662 (4)	0.8560 (4)	0.0503 (12)
C12	0.6580 (5)	0.4229 (4)	0.8529 (3)	0.0400 (10)
C13	0.5914 (6)	0.3516 (4)	0.6489 (3)	0.0443 (11)
C14	0.6707 (6)	0.2476 (5)	0.5775 (3)	0.0494 (12)
C15	0.8375 (9)	0.2381 (8)	0.6378 (5)	0.084 (2)

C16	0.7363 (6)	0.2971 (5)	0.4743 (3)	0.0507 (14)
C17	0.4856 (8)	0.1292 (5)	0.3288 (5)	0.0709 (17)
C18	0.6669 (8)	0.3653 (6)	0.3094 (4)	0.0664 (16)
Cl1	0.22428 (14)	0.32837 (11)	0.44260 (9)	0.0524 (3)
H2A	0.25720	0.17110	0.61670	0.0590*
H2B	0.50060	0.31300	0.42450	0.0540*
H3A	0.00520	−0.01930	0.63590	0.0660*
H4A	−0.00980	−0.10460	0.79140	0.0710*
H5A	0.23360	−0.00030	0.93150	0.0610*
H8A	0.77010	0.45550	1.11530	0.0600*
H9A	0.91380	0.68960	1.11470	0.0650*
H10A	0.90310	0.75580	0.95170	0.0650*
H11A	0.74180	0.59690	0.79220	0.0600*
H13A	0.68010	0.44670	0.65870	0.0530*
H13B	0.47660	0.34550	0.61050	0.0530*
H14A	0.57280	0.15410	0.55540	0.0590*
H15A	0.79770	0.19790	0.69920	0.1250*
H15B	0.92950	0.33080	0.66460	0.1250*
H15C	0.89070	0.17960	0.58800	0.1250*
H16A	0.81350	0.39620	0.49720	0.0610*
H16B	0.81480	0.24610	0.44000	0.0610*
H17A	0.41330	0.07910	0.37840	0.1060*
H17B	0.57500	0.08670	0.30100	0.1060*
H17C	0.40390	0.12520	0.26810	0.1060*
H18A	0.72400	0.46260	0.34880	0.0990*
H18B	0.56930	0.35570	0.25570	0.0990*
H18C	0.75940	0.33290	0.27250	0.0990*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0587 (6)	0.0433 (5)	0.0309 (5)	0.0145 (4)	−0.0028 (4)	0.0112 (3)
O1	0.095 (2)	0.0633 (19)	0.0316 (15)	0.0125 (17)	−0.0023 (15)	0.0187 (13)
O2	0.0562 (17)	0.0536 (17)	0.069 (2)	0.0230 (14)	−0.0042 (15)	0.0155 (15)
N1	0.0551 (18)	0.0425 (16)	0.0297 (15)	0.0128 (14)	0.0014 (13)	0.0101 (12)
N2	0.0564 (18)	0.0517 (18)	0.0292 (15)	0.0247 (15)	0.0070 (13)	0.0070 (12)
C1	0.0470 (19)	0.0416 (18)	0.0321 (17)	0.0179 (15)	0.0046 (14)	0.0063 (14)
C2	0.058 (2)	0.053 (2)	0.0380 (19)	0.0230 (18)	−0.0036 (17)	0.0090 (16)
C3	0.048 (2)	0.051 (2)	0.058 (3)	0.0115 (17)	−0.0092 (18)	0.0070 (19)
C4	0.052 (2)	0.050 (2)	0.068 (3)	0.0080 (18)	0.001 (2)	0.017 (2)
C5	0.056 (2)	0.047 (2)	0.048 (2)	0.0138 (17)	0.0061 (18)	0.0143 (17)
C6	0.0487 (19)	0.0388 (17)	0.0350 (18)	0.0151 (15)	0.0026 (14)	0.0075 (14)
C7	0.052 (2)	0.0384 (18)	0.0298 (17)	0.0134 (15)	0.0039 (14)	0.0059 (13)
C8	0.059 (2)	0.052 (2)	0.0287 (18)	0.0134 (18)	−0.0002 (16)	0.0028 (15)
C9	0.062 (2)	0.050 (2)	0.041 (2)	0.0147 (19)	0.0038 (18)	−0.0018 (17)
C10	0.062 (2)	0.0389 (19)	0.052 (2)	0.0098 (17)	0.0027 (19)	0.0066 (17)
C11	0.062 (2)	0.044 (2)	0.044 (2)	0.0167 (18)	0.0038 (17)	0.0124 (16)
C12	0.0455 (18)	0.0410 (18)	0.0327 (17)	0.0156 (15)	0.0041 (14)	0.0074 (14)

C13	0.058 (2)	0.048 (2)	0.0305 (17)	0.0195 (17)	0.0049 (15)	0.0152 (15)
C14	0.057 (2)	0.061 (2)	0.040 (2)	0.0286 (19)	0.0092 (17)	0.0195 (18)
C15	0.082 (3)	0.145 (6)	0.068 (3)	0.072 (4)	0.026 (3)	0.060 (4)
C16	0.052 (2)	0.071 (3)	0.037 (2)	0.029 (2)	0.0118 (16)	0.0172 (18)
C17	0.080 (3)	0.054 (3)	0.067 (3)	0.022 (2)	−0.006 (3)	−0.004 (2)
C18	0.086 (3)	0.084 (3)	0.040 (2)	0.036 (3)	0.020 (2)	0.026 (2)
Cl1	0.0493 (5)	0.0565 (6)	0.0514 (6)	0.0189 (4)	0.0047 (4)	0.0133 (4)

Geometric parameters (Å, º)

S1—O1	1.438 (3)	C14—C15	1.516 (9)
S1—O2	1.436 (3)	C14—C16	1.524 (6)
S1—C6	1.733 (4)	C2—H2A	0.9300
S1—C7	1.742 (4)	C3—H3A	0.9300
N1—C1	1.396 (5)	C4—H4A	0.9300
N1—C12	1.394 (5)	C5—H5A	0.9300
N1—C13	1.473 (5)	C8—H8A	0.9300
N2—C16	1.488 (6)	C9—H9A	0.9300
N2—C17	1.491 (7)	C10—H10A	0.9300
N2—C18	1.496 (7)	C11—H11A	0.9300
N2—H2B	0.9100	C13—H13A	0.9700
C1—C6	1.400 (5)	C13—H13B	0.9700
C1—C2	1.417 (6)	C14—H14A	0.9800
C2—C3	1.389 (7)	C15—H15A	0.9600
C3—C4	1.384 (7)	C15—H15B	0.9600
C4—C5	1.379 (7)	C15—H15C	0.9600
C5—C6	1.400 (6)	C16—H16A	0.9700
C7—C8	1.400 (5)	C16—H16B	0.9700
C7—C12	1.401 (5)	C17—H17A	0.9600
C8—C9	1.373 (6)	C17—H17B	0.9600
C9—C10	1.378 (7)	C17—H17C	0.9600
C10—C11	1.380 (7)	C18—H18A	0.9600
C11—C12	1.406 (6)	C18—H18B	0.9600
C13—C14	1.530 (6)	C18—H18C	0.9600
O1—S1—O2	117.1 (2)	C3—C4—H4A	120.00
O1—S1—C6	111.1 (2)	C5—C4—H4A	120.00
O1—S1—C7	110.2 (2)	C4—C5—H5A	120.00
O2—S1—C6	108.2 (2)	C6—C5—H5A	120.00
O2—S1—C7	108.99 (19)	C7—C8—H8A	120.00
C6—S1—C7	99.90 (19)	C9—C8—H8A	120.00
C1—N1—C12	121.7 (3)	C8—C9—H9A	121.00
C1—N1—C13	118.9 (3)	C10—C9—H9A	121.00
C12—N1—C13	119.3 (3)	C9—C10—H10A	119.00
C16—N2—C17	113.2 (4)	C11—C10—H10A	119.00
C16—N2—C18	109.4 (4)	C10—C11—H11A	119.00
C17—N2—C18	110.1 (4)	C12—C11—H11A	120.00
C16—N2—H2B	108.00	N1—C13—H13A	109.00

C17—N2—H2B	108.00	N1—C13—H13B	109.00
C18—N2—H2B	108.00	C14—C13—H13A	109.00
N1—C1—C2	120.7 (3)	C14—C13—H13B	109.00
N1—C1—C6	121.7 (4)	H13A—C13—H13B	108.00
C2—C1—C6	117.6 (4)	C13—C14—H14A	109.00
C1—C2—C3	119.4 (4)	C15—C14—H14A	109.00
C2—C3—C4	122.0 (4)	C16—C14—H14A	109.00
C3—C4—C5	119.6 (5)	C14—C15—H15A	109.00
C4—C5—C6	119.4 (4)	C14—C15—H15B	109.00
S1—C6—C1	118.3 (3)	C14—C15—H15C	110.00
S1—C6—C5	119.3 (3)	H15A—C15—H15B	109.00
C1—C6—C5	122.0 (4)	H15A—C15—H15C	109.00
C8—C7—C12	122.2 (4)	H15B—C15—H15C	110.00
S1—C7—C8	119.0 (3)	N2—C16—H16A	108.00
S1—C7—C12	118.6 (3)	N2—C16—H16B	108.00
C7—C8—C9	119.9 (4)	C14—C16—H16A	108.00
C8—C9—C10	118.8 (4)	C14—C16—H16B	108.00
C9—C10—C11	121.9 (4)	H16A—C16—H16B	107.00
C10—C11—C12	120.9 (4)	N2—C17—H17A	109.00
N1—C12—C7	121.2 (4)	N2—C17—H17B	110.00
N1—C12—C11	122.5 (4)	N2—C17—H17C	110.00
C7—C12—C11	116.2 (4)	H17A—C17—H17B	109.00
N1—C13—C14	112.6 (3)	H17A—C17—H17C	109.00
C13—C14—C15	112.2 (4)	H17B—C17—H17C	109.00
C13—C14—C16	109.1 (4)	N2—C18—H18A	109.00
C15—C14—C16	107.5 (4)	N2—C18—H18B	109.00
N2—C16—C14	115.8 (4)	N2—C18—H18C	109.00
C1—C2—H2A	120.00	H18A—C18—H18B	109.00
C3—C2—H2A	120.00	H18A—C18—H18C	110.00
C2—C3—H3A	119.00	H18B—C18—H18C	110.00
C4—C3—H3A	119.00		

O1—S1—C6—C1	154.8 (3)	C6—C1—C2—C3	2.2 (6)
O2—S1—C6—C1	−75.4 (4)	N1—C1—C2—C3	−176.5 (4)
C7—S1—C6—C1	38.5 (4)	N1—C1—C6—C5	175.2 (4)
O1—S1—C6—C5	−32.5 (4)	C2—C1—C6—S1	169.0 (3)
O2—S1—C6—C5	97.4 (4)	C2—C1—C6—C5	−3.5 (6)
C7—S1—C6—C5	−148.7 (3)	C1—C2—C3—C4	−0.1 (7)
O1—S1—C7—C8	30.5 (4)	C2—C3—C4—C5	−0.8 (7)
O2—S1—C7—C8	−99.3 (4)	C3—C4—C5—C6	−0.5 (7)
C6—S1—C7—C8	147.4 (4)	C4—C5—C6—C1	2.7 (7)
O1—S1—C7—C12	−154.8 (3)	C4—C5—C6—S1	−169.7 (4)
O2—S1—C7—C12	75.5 (4)	S1—C7—C12—C11	−172.2 (3)
C6—S1—C7—C12	−37.8 (4)	S1—C7—C12—N1	10.6 (5)
C12—N1—C13—C14	113.2 (4)	C12—C7—C8—C9	−2.4 (7)
C13—N1—C1—C2	−22.4 (6)	S1—C7—C8—C9	172.2 (4)
C12—N1—C1—C6	−24.9 (6)	C8—C7—C12—C11	2.4 (6)
C12—N1—C1—C2	153.8 (4)	C8—C7—C12—N1	−174.9 (4)

C1—N1—C13—C14	−70.6 (5)	C7—C8—C9—C10	0.3 (7)
C13—N1—C12—C7	−158.2 (4)	C8—C9—C10—C11	1.7 (7)
C13—N1—C1—C6	159.0 (4)	C9—C10—C11—C12	−1.6 (7)
C1—N1—C12—C7	25.7 (6)	C10—C11—C12—C7	−0.4 (6)
C1—N1—C12—C11	−151.4 (4)	C10—C11—C12—N1	176.8 (4)
C13—N1—C12—C11	24.8 (6)	N1—C13—C14—C15	−51.8 (6)
C18—N2—C16—C14	165.0 (4)	N1—C13—C14—C16	−170.8 (4)
C17—N2—C16—C14	−71.7 (5)	C15—C14—C16—N2	165.3 (4)
N1—C1—C6—S1	−12.3 (5)	C13—C14—C16—N2	−72.9 (5)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···Cl1	0.91	2.18	3.027 (4)	155
C13—H13*A*···Cl1^{i}	0.97	2.80	3.608 (4)	141
C13—H13*B*···Cl1	0.97	2.76	3.692 (4)	161
C17—H17*B*···*Cg*2^{ii}	0.96	2.62	3.559 (6)	166

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*, −*z*+1.