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3,11-Dibromo-14-(4-chlorophenyl)-14*H*-dibenzo[*a*,*j*]xanthene dimethylformamide monosolvate

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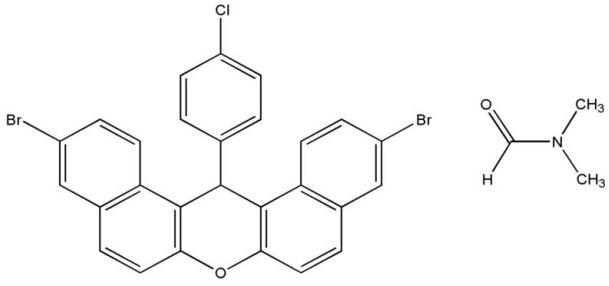
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.039; wR factor = 0.091; data-to-parameter ratio = 11.6.

In the title compound, $C_{27}H_{15}Br_2ClO\cdot C_3H_7NO$, the xanthene moiety has a flattened boat conformation with a folding angle between the naphthalene units of 9.46 (3)°. The mean planes of the xanthene system and its 4-chlorophenyl substituent are nearly perpendicular [dihedral angle = 89.43 (5)°]. The dimethylformamide solvent molecule is disordered over two sets of sites with an occupancy ratio of 0.520 (11):0.480 (11).

Related literature

For related structures and the preparation of the title compound, see: Wu *et al.* (2009); Seethalakshmi *et al.* (2006). For the biological activity of benzoxanthene derivatives, see: Lambert *et al.* (1997); Hideo (1981); Poupelin *et al.* (1978). For related structures, see: Cai *et al.* (2009); Lu *et al.* (2008); Rahmani *et al.* (2009); Dalla Via *et al.* (2008); Gaurrand *et al.* (2006); Petit *et al.* (2007).



Experimental

Crystal data

$C_{27}H_{15}Br_2ClO\cdot C_3H_7NO$
M_r = 623.74
Triclinic, $P\overline{1}$
a = 10.8558 (12) Å
b = 10.9385 (12) Å
c = 11.8946 (13) Å
α = 74.443 (1)°
β = 80.967 (1)°
γ = 71.448 (1)°
V = 1286.0 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.29 mm^{-1}
T = 293 K
0.28 × 0.26 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.415, T_{max} = 0.518
8696 measured reflections
4522 independent reflections
2902 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.091
S = 1.03
4522 reflections
375 parameters
55 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank Zhanhua Su for help with the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2054).

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supplementary materials

Acta Cryst. (2012). E**68**, o1460 [doi:10.1107/S1600536812016200]

3,11-Dibromo-14-(4-chlorophenyl)-14*H*-dibenzo[*a,j*]xanthene dimethylformamide monosolvate

Yong Bin Song and Bo Liu

Comment

Derivatives of benzoxanthenes have received much attention due to their wide range of biological and pharmacological activities, such as antiviral (Lambert *et al.*, 1997), antibacterial (Hideo, 1981), and anti-inflammatory (Poupelin *et al.*, 1978). In the present paper we describe the crystal structure of the title compound.

The molecular structure of the compound is shown in the Figure 1. The chlorophenyl substituent (C12–C17) at C11 forms dihedral angle of 89.43 (5)° with the mean plane of the xanthene ring system. The pyran ring (O1/C9/C10/C11/C18/C19) adopts a boat conformation with the O1 and C11 displaced by 0.112 and 0.253 (4) Å, respectively, from the mean plane of the rest of the atoms.

The packing is characterized by Cl···Br contacts and $\pi\cdots\pi$ stacking interactions. The distance between the Cl and Br atoms is 3.5668 (9) Å; The angles C1—Br1···Cl1 and C15—Cl1···Br1 are 161.43 (1)° and 85.97 (1)°, respectively. Some $\pi\cdots\pi$ stacking interactions between phenyl rings (containing Br1 and Br2, respectively) were detected with the centroid-to-centroid distance of 3.688 (2) Å. Short C-H···O contacts take place between the title molecule and the solvent.

Experimental

A solution of the 6-bromo-2-naphthol (2.2 g, 10 mmol), and 4-chloro-benzaldehyde (0.7 g, 5 mmol), acetic acid (5 ml) was refluxed with 1 ml of hydrochloric acid for two hours (Wu *et al.*, 2009). The system was cooled to room temperature, and the formed precipitate was filtered and washed with water. The product was recrystallized from the mixed solution of ethanol and dimethylformamide (DMF), and yielded raw crystals (2.2 g, yield 81%). The colourless single crystals of the title compound were grown by recystallization from DMF solution.

Refinement

The solvate DMF molecule is disordered over two positions. H atoms were positioned geometrically [C—H = 0.93 Å for aromatic ring, C—H = 0.98 Å for methenyl group, C—H = 0.93 Å for aldehyde group (DMF) and C—H = 0.96 Å for methyl group (DMF)] and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl and x = 1.2 for all other H atoms. Positions of H atoms of Me groups were optimized rotationally.

Computing details

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

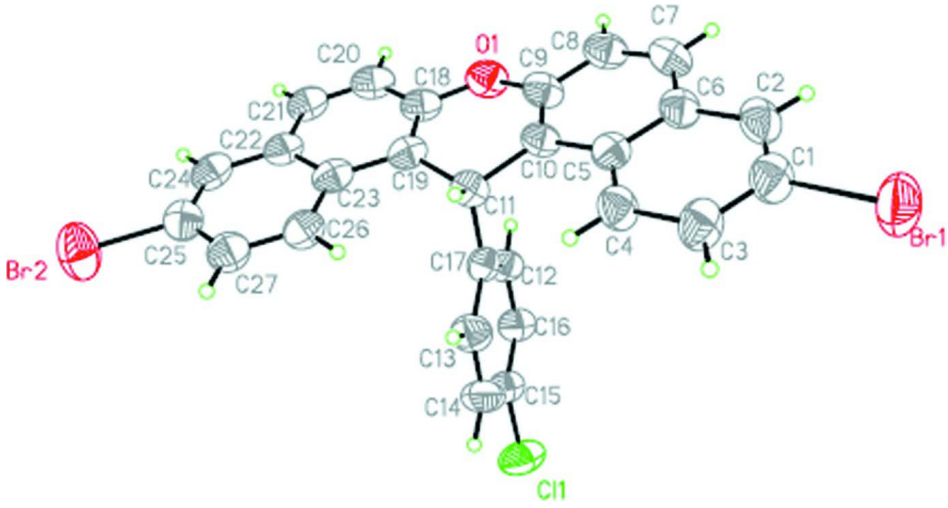

Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. The solvent molecule have been omitted for clarity.

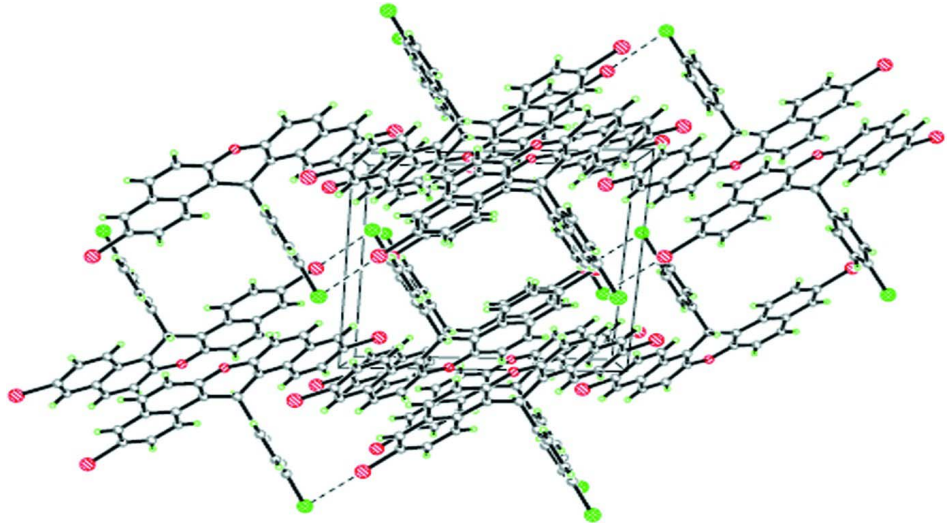

Figure 2

The crystal packing of the title compound viewed along the *b* axis. The solvent molecules have been omitted for clarity. Short Cl···Br contacts are shown by dashed lines (see Comments).

3,11-Dibromo-14-(4-chlorophenyl)-14*H*-dibenzo[*a*,*j*]xanthene dimethylformamide monosolvate

Crystal data

$C_{27}H_{15}Br_2ClO\cdot C_3H_7NO$
$M_r = 623.74$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.8558\ (12)$ Å
$b = 10.9385\ (12)$ Å
$c = 11.8946\ (13)$ Å
$\alpha = 74.443\ (1)°$
$\beta = 80.967\ (1)°$
$\gamma = 71.448\ (1)°$
$V = 1286.0\ (2)$ Å^3
$Z = 2$
$F(000) = 624.0$
$D_x = 1.611$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2346 reflections
$\theta = 2.4–23.0°$
$\mu = 3.29$ mm^{-1}

T = 293 K
Block, colourless

0.28 × 0.26 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.415, T_{max} = 0.518

8696 measured reflections
4522 independent reflections
2902 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°, θ_{min} = 2.4°
h = 12→12
k = 13→13
l = 14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.091
S = 1.03
4522 reflections
375 parameters
55 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
$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 0.0361P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.52851 (4)	0.29861 (5)	0.12824 (4)	0.08221 (18)	
Br2	1.12806 (5)	−0.43299 (4)	1.11655 (4)	0.08279 (18)	
Cl1	0.34543 (9)	0.24873 (11)	0.92900 (9)	0.0742 (3)	
C1	0.6372 (3)	0.2652 (4)	0.2508 (3)	0.0561 (9)	
C2	0.7071 (4)	0.3483 (4)	0.2477 (3)	0.0568 (10)	
H2	0.7036	0.4213	0.1850	0.068*	
C3	0.6406 (3)	0.1539 (4)	0.3421 (3)	0.0565 (9)	
H3	0.5926	0.0973	0.3412	0.068*	
C4	0.7150 (3)	0.1283 (3)	0.4333 (3)	0.0508 (9)	
H4	0.7166	0.0541	0.4943	0.061*	
C5	0.7893 (3)	0.2122 (3)	0.4366 (3)	0.0440 (8)	
C6	0.7857 (3)	0.3240 (3)	0.3399 (3)	0.0508 (9)	
C7	0.8624 (4)	0.4075 (4)	0.3393 (3)	0.0587 (10)	
H7	0.8626	0.4792	0.2761	0.070*	
C8	0.9352 (4)	0.3849 (4)	0.4288 (3)	0.0571 (10)	

H8	0.9860	0.4400	0.4267	0.068*	
C9	0.9339 (3)	0.2778 (4)	0.5253 (3)	0.0507 (9)	
C10	0.8637 (3)	0.1914 (3)	0.5327 (3)	0.0443 (8)	
C11	0.8579 (3)	0.0831 (3)	0.6435 (3)	0.0438 (8)	
H11	0.8662	0.0007	0.6211	0.053*	
C12	0.7273 (3)	0.1214 (3)	0.7159 (3)	0.0394 (7)	
C13	0.6464 (3)	0.0415 (3)	0.7511 (3)	0.0517 (9)	
H13	0.6697	−0.0390	0.7295	0.062*	
C14	0.5302 (3)	0.0793 (4)	0.8187 (3)	0.0591 (10)	
H14	0.4768	0.0238	0.8432	0.071*	
C15	0.4951 (3)	0.1983 (4)	0.8487 (3)	0.0477 (8)	
C16	0.5733 (3)	0.2804 (3)	0.8162 (3)	0.0505 (9)	
H16	0.5489	0.3611	0.8375	0.061*	
C17	0.6901 (3)	0.2400 (3)	0.7506 (3)	0.0480 (8)	
H17	0.7448	0.2942	0.7294	0.058*	
C18	1.0316 (3)	0.1546 (3)	0.7020 (3)	0.0476 (8)	
C19	0.9692 (3)	0.0601 (3)	0.7161 (3)	0.0432 (8)	
C20	1.1238 (3)	0.1442 (4)	0.7777 (3)	0.0547 (9)	
H20	1.1634	0.2111	0.7652	0.066*	
C21	1.1551 (3)	0.0378 (4)	0.8683 (3)	0.0509 (9)	
H21	1.2141	0.0331	0.9193	0.061*	
C22	1.0987 (3)	−0.0661 (3)	0.8857 (3)	0.0449 (8)	
C23	1.0052 (3)	−0.0563 (3)	0.8097 (3)	0.0441 (8)	
C24	1.1331 (3)	−0.1794 (4)	0.9783 (3)	0.0517 (9)	
H24	1.1934	−0.1859	1.0288	0.062*	
C25	1.0783 (3)	−0.2792 (3)	0.9939 (3)	0.0520 (9)	
C26	0.9516 (3)	−0.1635 (3)	0.8306 (3)	0.0486 (8)	
H26	0.8905	−0.1592	0.7819	0.058*	
C27	0.9868 (3)	−0.2727 (3)	0.9200 (3)	0.0529 (9)	
H27	0.9504	−0.3419	0.9318	0.063*	
O1S	0.2639 (19)	0.1711 (15)	0.4104 (17)	0.146 (7)	0.480 (11)
N1S	0.336 (3)	0.321 (2)	0.464 (3)	0.067 (4)	0.480 (11)
C1S	0.2884 (11)	0.2997 (12)	0.3778 (11)	0.080 (3)	0.480 (11)
H1S	0.2724	0.3592	0.3057	0.096*	0.480 (11)
C2S	0.3677 (10)	0.2212 (13)	0.5620 (9)	0.091 (4)	0.480 (11)
H2SA	0.2894	0.2086	0.6071	0.136*	0.480 (11)
H2SB	0.4180	0.2444	0.6083	0.136*	0.480 (11)
H2SC	0.4179	0.1406	0.5394	0.136*	0.480 (11)
C3S	0.3956 (14)	0.4246 (12)	0.4441 (14)	0.107 (4)	0.480 (11)
H3SA	0.3941	0.4703	0.3630	0.160*	0.480 (11)
H3SB	0.4842	0.3873	0.4646	0.160*	0.480 (11)
H3SC	0.3485	0.4858	0.4915	0.160*	0.480 (11)
O1	1.0076 (2)	0.2689 (2)	0.6136 (2)	0.0576 (6)	
O1Q	0.2462 (12)	0.226 (2)	0.3776 (18)	0.174 (9)	0.520 (11)
N1Q	0.349 (3)	0.315 (3)	0.463 (3)	0.070 (4)	0.520 (11)
C1Q	0.3174 (14)	0.2003 (14)	0.4823 (11)	0.128 (5)	0.520 (11)
H1Q	0.3355	0.1260	0.5443	0.153*	0.520 (11)
C2Q	0.3047 (14)	0.4214 (14)	0.3741 (10)	0.147 (8)	0.520 (11)
H2QA	0.2946	0.3914	0.3082	0.221*	0.520 (11)

H2QB	0.3659	0.4722	0.3518	0.221*	0.520 (11)
H2QC	0.2220	0.4758	0.3994	0.221*	0.520 (11)
C3Q	0.4112 (14)	0.336 (2)	0.5499 (17)	0.196 (11)	0.520 (11)
H3QA	0.4956	0.2722	0.5586	0.294*	0.520 (11)
H3QB	0.3592	0.3261	0.6231	0.294*	0.520 (11)
H3QC	0.4208	0.4239	0.5269	0.294*	0.520 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0733 (3)	0.1133 (4)	0.0549 (3)	−0.0121 (3)	−0.0207 (2)	−0.0202 (2)
Br2	0.1060 (4)	0.0687 (3)	0.0758 (3)	−0.0264 (3)	−0.0362 (3)	−0.0026 (2)
Cl1	0.0487 (6)	0.1130 (9)	0.0696 (7)	−0.0302 (6)	0.0088 (5)	−0.0353 (6)
C1	0.057 (2)	0.070 (3)	0.039 (2)	−0.005 (2)	−0.0072 (17)	−0.023 (2)
C2	0.063 (2)	0.060 (2)	0.038 (2)	−0.007 (2)	0.0002 (17)	−0.0135 (18)
C3	0.062 (2)	0.065 (3)	0.049 (2)	−0.0176 (19)	−0.0057 (18)	−0.024 (2)
C4	0.056 (2)	0.056 (2)	0.044 (2)	−0.0175 (18)	−0.0070 (16)	−0.0140 (17)
C5	0.0429 (19)	0.053 (2)	0.0359 (19)	−0.0108 (16)	0.0036 (14)	−0.0176 (16)
C6	0.049 (2)	0.056 (2)	0.044 (2)	−0.0094 (18)	0.0044 (16)	−0.0184 (18)
C7	0.070 (3)	0.057 (2)	0.046 (2)	−0.024 (2)	0.0081 (19)	−0.0097 (18)
C8	0.063 (2)	0.064 (2)	0.051 (2)	−0.030 (2)	0.0061 (19)	−0.017 (2)
C9	0.053 (2)	0.063 (2)	0.043 (2)	−0.0222 (19)	0.0017 (16)	−0.0205 (18)
C10	0.0443 (19)	0.050 (2)	0.041 (2)	−0.0149 (16)	0.0063 (15)	−0.0176 (16)
C11	0.0455 (19)	0.049 (2)	0.045 (2)	−0.0199 (16)	−0.0032 (15)	−0.0172 (16)
C12	0.0409 (18)	0.048 (2)	0.0365 (18)	−0.0180 (16)	−0.0092 (14)	−0.0109 (15)
C13	0.053 (2)	0.053 (2)	0.059 (2)	−0.0250 (18)	−0.0058 (17)	−0.0171 (18)
C14	0.048 (2)	0.078 (3)	0.061 (2)	−0.036 (2)	0.0011 (18)	−0.015 (2)
C15	0.0389 (19)	0.068 (2)	0.040 (2)	−0.0186 (18)	−0.0036 (14)	−0.0161 (18)
C16	0.052 (2)	0.058 (2)	0.047 (2)	−0.0193 (18)	−0.0018 (16)	−0.0182 (17)
C17	0.045 (2)	0.058 (2)	0.047 (2)	−0.0249 (17)	−0.0014 (16)	−0.0119 (17)
C18	0.044 (2)	0.056 (2)	0.051 (2)	−0.0202 (18)	0.0009 (16)	−0.0225 (18)
C19	0.0373 (18)	0.054 (2)	0.044 (2)	−0.0141 (16)	−0.0022 (14)	−0.0193 (17)
C20	0.048 (2)	0.068 (3)	0.062 (3)	−0.0268 (19)	−0.0010 (18)	−0.028 (2)
C21	0.040 (2)	0.067 (2)	0.056 (2)	−0.0183 (18)	−0.0060 (16)	−0.028 (2)
C22	0.0354 (18)	0.059 (2)	0.046 (2)	−0.0136 (17)	0.0002 (15)	−0.0223 (18)
C23	0.0359 (18)	0.054 (2)	0.048 (2)	−0.0112 (16)	0.0036 (15)	−0.0261 (17)
C24	0.041 (2)	0.068 (2)	0.049 (2)	−0.0086 (18)	−0.0058 (15)	−0.0255 (19)
C25	0.055 (2)	0.052 (2)	0.049 (2)	−0.0109 (18)	−0.0051 (17)	−0.0147 (17)
C26	0.045 (2)	0.053 (2)	0.053 (2)	−0.0129 (17)	−0.0094 (16)	−0.0198 (18)
C27	0.050 (2)	0.056 (2)	0.056 (2)	−0.0157 (18)	−0.0043 (17)	−0.0184 (19)
O1S	0.219 (18)	0.105 (8)	0.152 (11)	−0.095 (10)	0.051 (10)	−0.071 (7)
N1S	0.066 (10)	0.033 (6)	0.091 (9)	0.000 (6)	0.001 (7)	−0.017 (5)
C1S	0.066 (6)	0.090 (7)	0.071 (5)	−0.016 (5)	−0.004 (4)	−0.008 (5)
C2S	0.088 (6)	0.121 (8)	0.061 (6)	−0.047 (6)	−0.009 (5)	0.005 (5)
C3S	0.111 (8)	0.089 (7)	0.124 (9)	−0.039 (6)	0.024 (7)	−0.038 (6)
O1	0.0637 (16)	0.0636 (16)	0.0566 (16)	−0.0333 (13)	−0.0057 (12)	−0.0140 (13)
O1Q	0.058 (6)	0.28 (2)	0.247 (18)	−0.025 (9)	0.000 (8)	−0.201 (17)
N1Q	0.063 (7)	0.087 (8)	0.063 (6)	−0.032 (6)	−0.003 (5)	−0.009 (6)
C1Q	0.157 (12)	0.112 (9)	0.119 (11)	−0.055 (8)	0.039 (8)	−0.045 (8)

C2Q	0.137 (11)	0.118 (10)	0.084 (8)	0.045 (9)	0.023 (7)	0.029 (7)
C3Q	0.126 (11)	0.26 (2)	0.236 (19)	0.050 (12)	−0.093 (12)	−0.191 (18)

Geometric parameters (Å, º)

Br1—C1	1.906 (4)	C19—C23	1.440 (4)
Br2—C25	1.898 (3)	C20—C21	1.350 (4)
Cl1—C15	1.756 (3)	C20—H20	0.9300
C1—C2	1.346 (5)	C21—C22	1.410 (4)
C1—C3	1.392 (5)	C21—H21	0.9300
C2—C6	1.413 (5)	C22—C24	1.411 (4)
C2—H2	0.9300	C22—C23	1.424 (4)
C3—C4	1.370 (5)	C23—C26	1.416 (4)
C3—H3	0.9300	C24—C25	1.360 (5)
C4—C5	1.413 (4)	C24—H24	0.9300
C4—H4	0.9300	C25—C27	1.400 (5)
C5—C10	1.429 (4)	C26—C27	1.363 (4)
C5—C6	1.432 (4)	C26—H26	0.9300
C6—C7	1.416 (5)	C27—H27	0.9300
C7—C8	1.347 (5)	O1S—C1S	1.453 (17)
C7—H7	0.9300	N1S—C1S	1.32 (2)
C8—C9	1.406 (5)	N1S—C2S	1.37 (3)
C8—H8	0.9300	N1S—C3S	1.42 (2)
C9—C10	1.369 (4)	C1S—H1S	0.9300
C9—O1	1.383 (4)	C2S—H2SA	0.9600
C10—C11	1.527 (4)	C2S—H2SB	0.9600
C11—C19	1.512 (4)	C2S—H2SC	0.9600
C11—C12	1.536 (4)	C3S—H3SA	0.9600
C11—H11	0.9800	C3S—H3SB	0.9600
C12—C13	1.374 (4)	C3S—H3SC	0.9600
C12—C17	1.384 (4)	O1Q—C1Q	1.485 (18)
C13—C14	1.392 (5)	N1Q—C2Q	1.36 (3)
C13—H13	0.9300	N1Q—C1Q	1.36 (2)
C14—C15	1.363 (5)	N1Q—C3Q	1.42 (2)
C14—H14	0.9300	C1Q—H1Q	0.9300
C15—C16	1.369 (4)	C2Q—H2QA	0.9600
C16—C17	1.388 (4)	C2Q—H2QB	0.9600
C16—H16	0.9300	C2Q—H2QC	0.9600
C17—H17	0.9300	C3Q—H3QA	0.9600
C18—C19	1.368 (4)	C3Q—H3QB	0.9600
C18—O1	1.381 (4)	C3Q—H3QC	0.9600
C18—C20	1.408 (5)		
C2—C1—C3	122.1 (3)	C19—C18—C20	122.6 (3)
C2—C1—Br1	120.1 (3)	O1—C18—C20	114.6 (3)
C3—C1—Br1	117.8 (3)	C18—C19—C23	117.5 (3)
C1—C2—C6	119.7 (3)	C18—C19—C11	121.1 (3)
C1—C2—H2	120.1	C23—C19—C11	121.2 (3)
C6—C2—H2	120.1	C21—C20—C18	120.5 (3)
C4—C3—C1	119.5 (3)	C21—C20—H20	119.8

C4—C3—H3	120.2	C18—C20—H20	119.8
C1—C3—H3	120.2	C20—C21—C22	120.2 (3)
C3—C4—C5	121.4 (3)	C20—C21—H21	119.9
C3—C4—H4	119.3	C22—C21—H21	119.9
C5—C4—H4	119.3	C21—C22—C24	120.7 (3)
C4—C5—C10	122.8 (3)	C21—C22—C23	119.7 (3)
C4—C5—C6	117.4 (3)	C24—C22—C23	119.5 (3)
C10—C5—C6	119.8 (3)	C26—C23—C22	117.6 (3)
C2—C6—C7	121.7 (3)	C26—C23—C19	123.0 (3)
C2—C6—C5	119.7 (3)	C22—C23—C19	119.4 (3)
C7—C6—C5	118.6 (3)	C25—C24—C22	120.2 (3)
C8—C7—C6	121.2 (3)	C25—C24—H24	119.9
C8—C7—H7	119.4	C22—C24—H24	119.9
C6—C7—H7	119.4	C24—C25—C27	121.5 (3)
C7—C8—C9	119.6 (4)	C24—C25—Br2	119.8 (3)
C7—C8—H8	120.2	C27—C25—Br2	118.6 (3)
C9—C8—H8	120.2	C27—C26—C23	122.1 (3)
C10—C9—O1	122.8 (3)	C27—C26—H26	119.0
C10—C9—C8	123.1 (3)	C23—C26—H26	119.0
O1—C9—C8	114.1 (3)	C26—C27—C25	119.1 (3)
C9—C10—C5	117.6 (3)	C26—C27—H27	120.4
C9—C10—C11	120.8 (3)	C25—C27—H27	120.4
C5—C10—C11	121.4 (3)	C1S—N1S—C2S	119.2 (16)
C19—C11—C10	109.9 (3)	C1S—N1S—C3S	121 (3)
C19—C11—C12	109.9 (3)	C2S—N1S—C3S	116.1 (18)
C10—C11—C12	110.6 (3)	N1S—C1S—O1S	111.3 (17)
C19—C11—H11	108.8	N1S—C1S—H1S	124.3
C10—C11—H11	108.8	O1S—C1S—H1S	124.3
C12—C11—H11	108.8	C18—O1—C9	118.2 (3)
C13—C12—C17	117.9 (3)	C2Q—N1Q—C1Q	123.1 (17)
C13—C12—C11	123.0 (3)	C2Q—N1Q—C3Q	116.9 (19)
C17—C12—C11	119.1 (3)	C1Q—N1Q—C3Q	119 (2)
C12—C13—C14	120.9 (3)	N1Q—C1Q—O1Q	100.8 (16)
C12—C13—H13	119.5	N1Q—C1Q—H1Q	129.6
C14—C13—H13	119.5	O1Q—C1Q—H1Q	129.6
C15—C14—C13	119.5 (3)	N1Q—C2Q—H2QA	109.5
C15—C14—H14	120.3	N1Q—C2Q—H2QB	109.5
C13—C14—H14	120.3	H2QA—C2Q—H2QB	109.5
C14—C15—C16	121.4 (3)	N1Q—C2Q—H2QC	109.5
C14—C15—Cl1	119.4 (3)	H2QA—C2Q—H2QC	109.5
C16—C15—Cl1	119.1 (3)	H2QB—C2Q—H2QC	109.5
C15—C16—C17	118.3 (3)	N1Q—C3Q—H3QA	109.5
C15—C16—H16	120.8	N1Q—C3Q—H3QB	109.5
C17—C16—H16	120.8	H3QA—C3Q—H3QB	109.5
C12—C17—C16	121.9 (3)	N1Q—C3Q—H3QC	109.5
C12—C17—H17	119.1	H3QA—C3Q—H3QC	109.5
C16—C17—H17	119.1	H3QB—C3Q—H3QC	109.5
C19—C18—O1	122.8 (3)		