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Propan-1-aminium 3,4,5,6-tetrabromo-2-(methoxycarbonyl)benzoate *N*,*N*-dimethylformamide monosolvate

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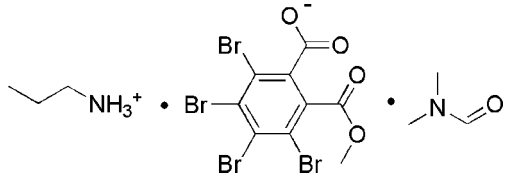
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; disorder in solvent or counterion; R factor = 0.047; wR factor = 0.104; data-to-parameter ratio = 14.3.

In the anion of the title solvated molecular salt, $C_3H_{10}N^+\cdot C_9H_3Br_4O_4^-\cdot C_3H_7NO$, the dihedral angles formed by the aromatic ring and the mean planes of the carboxylate and methoxycarbonyl groups are 64.3 (3) and 75.2 (3)°, respectively. The C atoms of the propan-1-aminium cation are disordered over two sets of sites in a 0.65 (3):0.35 (3) ratio. The crystal structure is stabilized by N—H···O hydrogen bonds.

Related literature

For related structures, see: Li (2011*a*,*b*).



Experimental

Crystal data

$C_3H_{10}N^+\cdot C_9H_3Br_4O_4^-\cdot C_3H_7NO$
M_r = 627.97
Monoclinic, $P2_1/n$
a = 11.8964 (11) Å
b = 10.5198 (10) Å
c = 17.3743 (17) Å
β = 93.188 (1)°
V = 2171.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.44 mm^{-1}
T = 298 K
0.40 × 0.37 × 0.24 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.155, T_{max} = 0.268
10672 measured reflections
3821 independent reflections
1836 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.104
S = 1.03
3821 reflections
268 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O3	0.89	1.87	2.757 (7)	175
N1—H1B···O4^{i}	0.89	2.04	2.812 (8)	144
N1—H1C···O5^{ii}	0.89	1.91	2.762 (8)	160

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, y-1, z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5538).

References

Bruker (1997). *SADABS*, *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, J. (2011*a*). *Acta Cryst.* E**67**, o200.
Li, J. (2011*b*). *Acta Cryst.* E**67**, o900.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, o1356 [doi:10.1107/S1600536811016850]

Propan-1-aminium 3,4,5,6-tetrabromo-2-(methoxycarbonyl)benzoate *N*,*N*-dimethylformamide monosolvate

Jian Li

S1. Comment

4,5,6,7-Tetrabromo-2-ethylisoindoline-1,3-dione is an important flame retardant. 3,4,5,6-Tetrabromo-2-(methoxycarbonyl)benzoic acid is an intermediate in the synthesis of this flame retardant. The asymmetric unit of the title compound contains one propan-1-aminium cation, one 3,4,5,6-tetrabromo-2-(methoxycarbonyl)benzoate anion and one *N*,*N*-dimethylformamide solvent molecule (Fig. 1). In the anion of the title compound, the dihedral angles formed by the benzene ring and the mean planes of the carboxylate and methoxycarbonyl groups are 64.3 (3) and 75.2 (3) °, respectively. The carbon atoms of the propan-1-aminium cation are disordered. The bond lengths and angles are in agreement with those which are related in ethylammonium 2-(methoxycarbonyl)-3,4,5,6-tetrabromobenzoate methanol solvate (Li, 2011*a*) and in 2-Methylanilinium 3,4,5,6-tetrabromo-2-(methoxycarbonyl)benzoate methanol monosolvate(Li, 2011*b*). The crystal structure is stabilized by N—H···O hydrogen bonds (see Fig. 2 and Table 1).

S2. Experimental

A mixture of 4,5,6,7-tetrabromoisobenzofuran-1,3-dione (4.64 g, 0.01 mol) and methanol (15 ml) was refluxed for 0.5 h. Then propan-1-amine (0.59 g, 0.01 mol) was added to the above solution and mixed for 30 min at room temperature. After filtration, filter cake was disolved in *N*,*N*-dimethylformamide (10 ml), the solution was kept at room temperature for 15 d. Natural evaporation gave colourless single crystals of the title compound, suitable for X-ray analysis.

S3. Refinement

H atoms were refined using a riding model with C—H = 0.96–0.97 Å, N—H = 0.89 Å, O—H = 0.82Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O, N, methyl C).

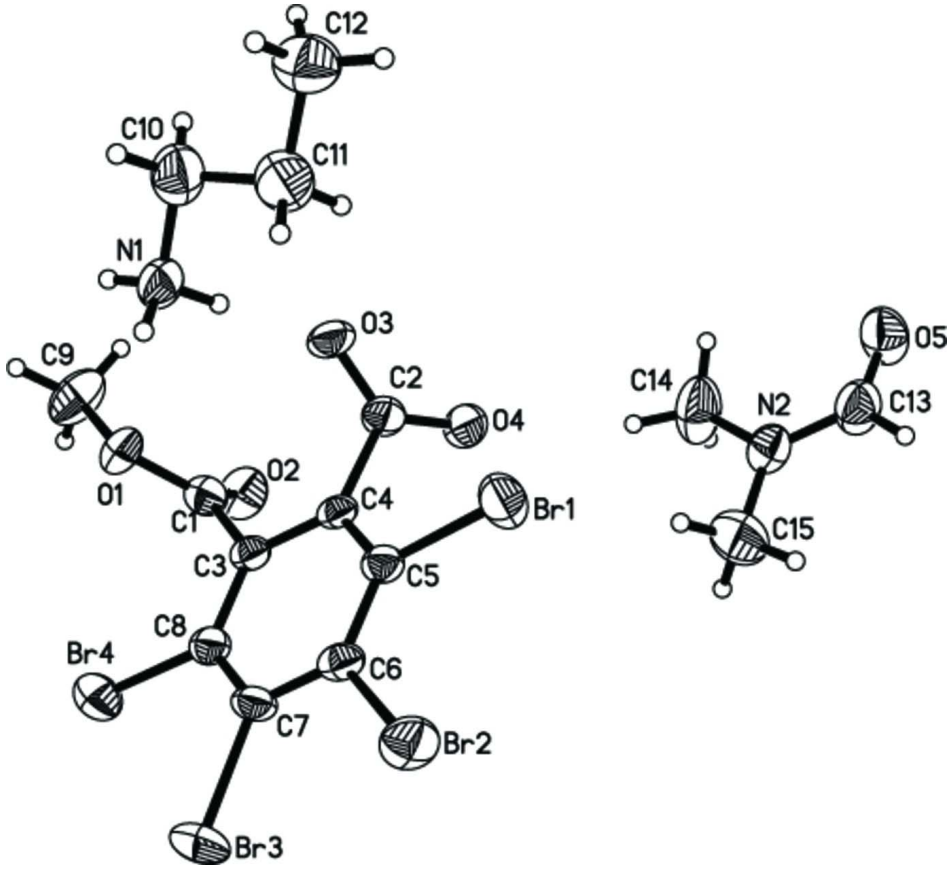

Figure 1

The molecular structure of the title compound drawn with 30% probability ellipsoids.

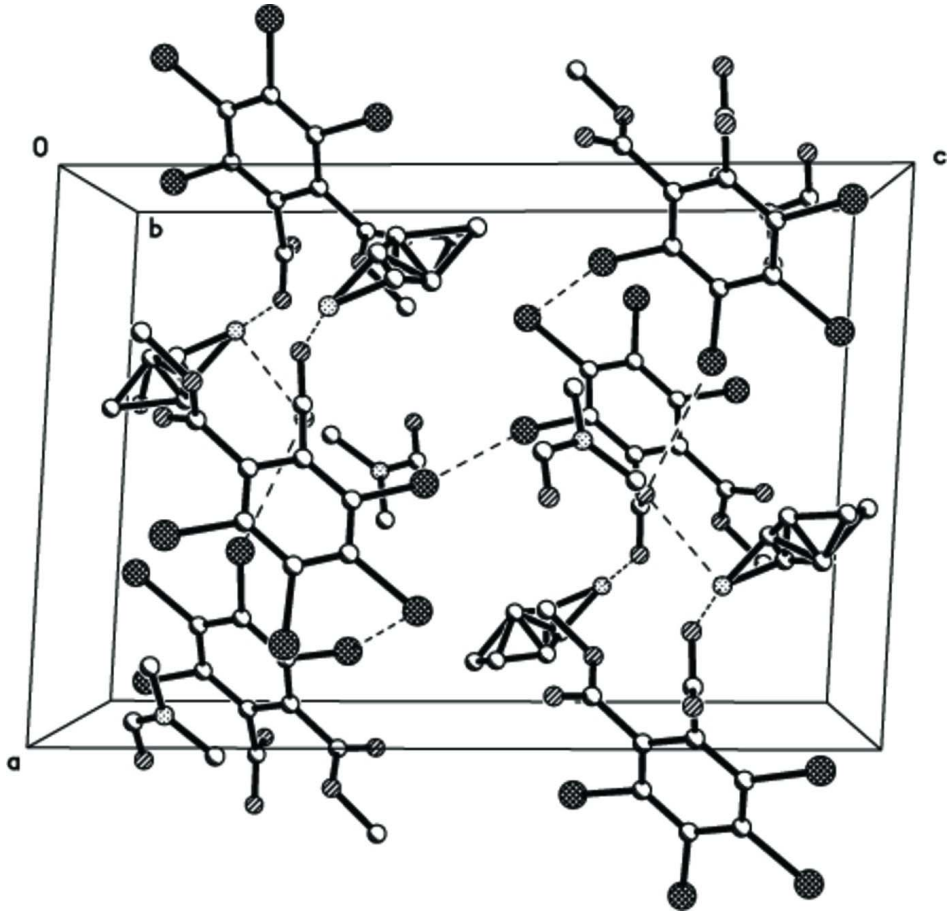

Figure 2

The crystal structure is stabilized by N—H···O hydrogen bonds

Propan-1-aminium 3,4,5,6-tetrabromo-2-(methoxycarbonyl)benzoate *N*,*N*-dimethylformamide monosolvate

Crystal data

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c = 17.3743 (17) Å
β = 93.188 (1)°
V = 2171.0 (4) Å^3
Z = 4
$F(000)$ = 1216
D_x = 1.921 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1875 reflections
θ = 2.3–20.1°
μ = 7.44 mm^{-1}
T = 298 K
Block, colorless
0.40 × 0.37 × 0.24 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.155, T_{max} = 0.268
10672 measured reflections
3821 independent reflections
1836 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −14→14
k = −12→12
l = −10→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.104$
$S = 1.03$
3821 reflections
268 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
$w = 1/[\sigma^2(F_o^2) + (0.0346P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.57$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ 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	0.54990 (6)	0.36358 (7)	0.43979 (5)	0.0768 (3)	
Br2	0.77382 (6)	0.18088 (8)	0.44525 (5)	0.0787 (3)	
Br3	0.82232 (6)	−0.00007 (9)	0.29589 (6)	0.0923 (3)	
Br4	0.63517 (6)	−0.01203 (8)	0.14923 (5)	0.0828 (3)	
N1	0.2391 (5)	0.0691 (6)	0.3225 (4)	0.0701 (18)	
H1A	0.2650	0.1457	0.3109	0.105*	0.65 (3)
H1B	0.2129	0.0305	0.2796	0.105*	0.65 (3)
H1C	0.2947	0.0231	0.3447	0.105*	0.65 (3)
H1′A	0.1918	0.0366	0.2862	0.105*	0.35 (3)
H1′B	0.3018	0.0227	0.3261	0.105*	0.35 (3)
H1′C	0.2560	0.1487	0.3102	0.105*	0.35 (3)
N2	0.5289 (5)	0.8141 (7)	0.3665 (4)	0.0697 (18)	
O1	0.3696 (4)	0.0717 (5)	0.1644 (3)	0.0631 (14)	
O2	0.4289 (4)	0.2556 (5)	0.1162 (3)	0.0776 (16)	
O3	0.3100 (3)	0.3064 (5)	0.2784 (3)	0.0721 (15)	
O4	0.4291 (4)	0.4662 (5)	0.2792 (3)	0.0740 (16)	
O5	0.4306 (5)	0.9836 (5)	0.4037 (3)	0.0917 (19)	
C1	0.4351 (6)	0.1731 (8)	0.1638 (4)	0.056 (2)	
C2	0.4049 (6)	0.3538 (7)	0.2822 (4)	0.0541 (19)	
C3	0.5206 (5)	0.1754 (6)	0.2302 (4)	0.0438 (17)	
C4	0.5034 (5)	0.2591 (6)	0.2915 (4)	0.0432 (17)	
C5	0.5786 (5)	0.2591 (6)	0.3546 (4)	0.0471 (18)	
C6	0.6718 (5)	0.1788 (7)	0.3581 (4)	0.0501 (18)	
C7	0.6908 (5)	0.1006 (6)	0.2960 (4)	0.0522 (19)	
C8	0.6138 (5)	0.0966 (6)	0.2343 (4)	0.0514 (19)	

C9	0.2842 (6)	0.0614 (8)	0.1018 (4)	0.092 (3)	
H9A	0.2345	0.1332	0.1029	0.138*	
H9B	0.2420	−0.0154	0.1075	0.138*	
H9C	0.3197	0.0597	0.0535	0.138*	
C10	0.146 (3)	0.082 (4)	0.377 (3)	0.092 (10)	0.65 (3)
H10A	0.1269	0.0002	0.3975	0.110*	0.65 (3)
H10B	0.0798	0.1186	0.3504	0.110*	0.65 (3)
C11	0.1904 (17)	0.169 (2)	0.4401 (13)	0.105 (8)	0.65 (3)
H11A	0.2540	0.1306	0.4687	0.125*	0.65 (3)
H11B	0.2141	0.2496	0.4192	0.125*	0.65 (3)
C12	0.0942 (16)	0.188 (3)	0.4911 (12)	0.109 (7)	0.65 (3)
H12A	0.0279	0.2109	0.4602	0.164*	0.65 (3)
H12B	0.1124	0.2546	0.5274	0.164*	0.65 (3)
H12C	0.0806	0.1106	0.5183	0.164*	0.65 (3)
C10′	0.191 (5)	0.079 (9)	0.398 (5)	0.091 (18)	0.35 (3)
H10C	0.2502	0.0933	0.4382	0.109*	0.35 (3)
H10D	0.1521	0.0006	0.4103	0.109*	0.35 (3)
C11′	0.110 (3)	0.190 (4)	0.394 (2)	0.099 (14)	0.35 (3)
H11C	0.1282	0.2414	0.3501	0.119*	0.35 (3)
H11D	0.0349	0.1553	0.3821	0.119*	0.35 (3)
C12′	0.103 (4)	0.275 (4)	0.461 (4)	0.120 (16)	0.35 (3)
H12D	0.1432	0.2385	0.5045	0.180*	0.35 (3)
H12E	0.0251	0.2863	0.4720	0.180*	0.35 (3)
H12F	0.1348	0.3560	0.4490	0.180*	0.35 (3)
C13	0.5086 (7)	0.9088 (9)	0.4133 (5)	0.084 (3)	
H13	0.5571	0.9195	0.4567	0.101*	
C14	0.4573 (7)	0.7909 (8)	0.2986 (5)	0.111 (3)	
H14A	0.3816	0.8159	0.3080	0.166*	
H14B	0.4587	0.7021	0.2862	0.166*	
H14C	0.4837	0.8393	0.2564	0.166*	
C15	0.6236 (7)	0.7288 (8)	0.3804 (6)	0.113 (3)	
H15A	0.6662	0.7546	0.4263	0.169*	
H15B	0.6709	0.7317	0.3374	0.169*	
H15C	0.5966	0.6437	0.3868	0.169*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0844 (6)	0.0688 (6)	0.0766 (6)	0.0133 (4)	−0.0017 (5)	−0.0155 (5)
Br2	0.0667 (5)	0.0806 (6)	0.0862 (7)	0.0101 (4)	−0.0205 (5)	0.0123 (5)
Br3	0.0556 (4)	0.0903 (7)	0.1302 (8)	0.0342 (5)	−0.0014 (5)	−0.0098 (6)
Br4	0.0749 (5)	0.0825 (6)	0.0923 (7)	0.0100 (5)	0.0163 (5)	−0.0266 (5)
N1	0.060 (4)	0.068 (4)	0.080 (5)	−0.008 (3)	−0.011 (4)	−0.011 (4)
N2	0.071 (4)	0.061 (4)	0.076 (5)	−0.011 (4)	−0.002 (4)	0.001 (4)
O1	0.057 (3)	0.063 (3)	0.068 (4)	−0.018 (3)	−0.009 (3)	0.002 (3)
O2	0.085 (4)	0.073 (4)	0.073 (4)	−0.007 (3)	−0.009 (3)	0.018 (3)
O3	0.034 (3)	0.057 (3)	0.124 (5)	0.003 (2)	−0.001 (3)	0.008 (3)
O4	0.055 (3)	0.038 (3)	0.128 (5)	0.003 (2)	−0.001 (3)	0.008 (3)

O5	0.098 (4)	0.076 (4)	0.097 (5)	0.026 (3)	−0.027 (4)	−0.012 (4)
C1	0.054 (4)	0.056 (6)	0.059 (6)	0.006 (4)	0.007 (4)	0.004 (5)
C2	0.045 (4)	0.054 (5)	0.062 (5)	0.007 (4)	−0.006 (4)	0.004 (4)
C3	0.035 (4)	0.044 (4)	0.053 (5)	−0.002 (3)	0.003 (4)	0.009 (4)
C4	0.030 (3)	0.042 (4)	0.057 (5)	−0.004 (3)	0.005 (4)	0.010 (4)
C5	0.039 (4)	0.045 (4)	0.058 (5)	0.002 (3)	0.001 (4)	0.006 (4)
C6	0.037 (4)	0.051 (4)	0.063 (5)	−0.002 (3)	0.004 (4)	0.014 (4)
C7	0.037 (4)	0.048 (5)	0.072 (6)	0.011 (3)	0.006 (4)	0.008 (4)
C8	0.042 (4)	0.041 (4)	0.071 (5)	0.000 (3)	0.007 (4)	0.010 (4)
C9	0.081 (5)	0.125 (7)	0.065 (6)	−0.034 (5)	−0.025 (5)	0.002 (6)
C10	0.09 (2)	0.078 (17)	0.11 (3)	0.005 (19)	−0.018 (18)	−0.008 (16)
C11	0.086 (13)	0.107 (17)	0.119 (17)	0.008 (11)	−0.011 (13)	−0.025 (14)
C12	0.099 (12)	0.12 (2)	0.107 (15)	−0.005 (15)	0.028 (11)	−0.008 (15)
C10′	0.08 (4)	0.09 (3)	0.10 (6)	0.01 (3)	−0.02 (3)	−0.01 (3)
C11′	0.08 (2)	0.11 (3)	0.11 (3)	0.01 (2)	−0.01 (2)	−0.01 (3)
C12′	0.12 (3)	0.08 (3)	0.15 (4)	0.01 (2)	0.00 (3)	−0.03 (3)
C13	0.083 (6)	0.078 (7)	0.088 (7)	0.002 (5)	−0.021 (6)	−0.011 (6)
C14	0.134 (8)	0.086 (7)	0.106 (8)	0.000 (6)	−0.046 (7)	−0.017 (6)
C15	0.096 (6)	0.093 (7)	0.149 (10)	0.032 (6)	−0.004 (6)	−0.011 (7)

Geometric parameters (Å, º)

Br1—C5	1.890 (7)	C9—H9A	0.9600
Br2—C6	1.887 (6)	C9—H9B	0.9600
Br3—C7	1.889 (6)	C9—H9C	0.9600
Br4—C8	1.897 (7)	C10—C11	1.50 (6)
N1—C10′	1.47 (10)	C10—H10A	0.9700
N1—C10	1.50 (5)	C10—H10B	0.9700
N1—H1A	0.8900	C11—C12	1.50 (2)
N1—H1B	0.8900	C11—H11A	0.9700
N1—H1C	0.8900	C11—H11B	0.9700
N1—H1′A	0.8900	C12—H12A	0.9600
N1—H1′B	0.8900	C12—H12B	0.9600
N1—H1′C	0.8900	C12—H12C	0.9600
N2—C13	1.318 (9)	C10′—C11′	1.52 (10)
N2—C14	1.436 (8)	C10′—H10C	0.9700
N2—C15	1.450 (9)	C10′—H10D	0.9700
O1—C1	1.322 (8)	C11′—C12′	1.47 (5)
O1—C9	1.451 (7)	C11′—H11C	0.9700
O2—C1	1.198 (7)	C11′—H11D	0.9700
O3—C2	1.232 (7)	C12′—H12D	0.9600
O4—C2	1.220 (7)	C12′—H12E	0.9600
O5—C13	1.221 (9)	C12′—H12F	0.9600
C1—C3	1.495 (9)	C13—H13	0.9300
C2—C4	1.539 (8)	C14—H14A	0.9600
C3—C8	1.383 (8)	C14—H14B	0.9600
C3—C4	1.406 (8)	C14—H14C	0.9600
C4—C5	1.375 (8)	C15—H15A	0.9600

C5—C6	1.393 (8)	C15—H15B	0.9600
C6—C7	1.386 (9)	C15—H15C	0.9600
C7—C8	1.371 (8)		

C10′—N1—C10	24.7 (18)	C7—C8—Br4	121.0 (5)
C10′—N1—H1A	107.3	C3—C8—Br4	117.5 (5)
C10—N1—H1A	109.5	O1—C9—H9A	109.5
C10′—N1—H1B	130.3	O1—C9—H9B	109.5
C10—N1—H1B	109.5	H9A—C9—H9B	109.5
H1A—N1—H1B	109.5	O1—C9—H9C	109.5
C10′—N1—H1C	87.9	H9A—C9—H9C	109.5
C10—N1—H1C	109.5	H9B—C9—H9C	109.5
H1A—N1—H1C	109.5	N1—C10—C11	106 (2)
H1B—N1—H1C	109.5	N1—C10—H10A	110.5
C10′—N1—H1′A	113.6	C11—C10—H10A	110.5
C10—N1—H1′A	91.3	N1—C10—H10B	110.5
H1A—N1—H1′A	113.6	C11—C10—H10B	110.5
H1B—N1—H1′A	18.7	H10A—C10—H10B	108.7
H1C—N1—H1′A	121.6	C12—C11—C10	105 (2)
C10′—N1—H1′B	109.9	C12—C11—H11A	110.6
C10—N1—H1′B	130.6	C10—C11—H11A	110.6
H1A—N1—H1′B	102.4	C12—C11—H11B	110.6
H1B—N1—H1′B	93.6	C10—C11—H11B	110.6
H1C—N1—H1′B	22.0	H11A—C11—H11B	108.8
H1′A—N1—H1′B	109.5	N1—C10′—C11′	106 (5)
C10′—N1—H1′C	104.9	N1—C10′—H10C	110.4
C10—N1—H1′C	104.3	C11′—C10′—H10C	110.4
H1A—N1—H1′C	7.2	N1—C10′—H10D	110.4
H1B—N1—H1′C	107.5	C11′—C10′—H10D	110.4
H1C—N1—H1′C	116.4	H10C—C10′—H10D	108.6
H1′A—N1—H1′C	109.5	C12′—C11′—C10′	119 (4)
H1′B—N1—H1′C	109.5	C12′—C11′—H11C	107.5
C13—N2—C14	121.0 (7)	C10′—C11′—H11C	107.5
C13—N2—C15	122.2 (8)	C12′—C11′—H11D	107.5
C14—N2—C15	116.9 (7)	C10′—C11′—H11D	107.5
C1—O1—C9	116.2 (6)	H11C—C11′—H11D	107.0
O2—C1—O1	125.3 (7)	C11′—C12′—H12D	109.5
O2—C1—C3	122.2 (7)	C11′—C12′—H12E	109.5
O1—C1—C3	112.5 (7)	H12D—C12′—H12E	109.5
O4—C2—O3	127.5 (6)	C11′—C12′—H12F	109.5
O4—C2—C4	116.8 (6)	H12D—C12′—H12F	109.5
O3—C2—C4	115.7 (6)	H12E—C12′—H12F	109.5
C8—C3—C4	119.1 (6)	O5—C13—N2	124.5 (8)
C8—C3—C1	122.7 (6)	O5—C13—H13	117.7
C4—C3—C1	118.2 (6)	N2—C13—H13	117.7
C5—C4—C3	119.2 (6)	N2—C14—H14A	109.5
C5—C4—C2	122.8 (6)	N2—C14—H14B	109.5
C3—C4—C2	117.9 (6)	H14A—C14—H14B	109.5

C4—C5—C6	121.1 (6)	N2—C14—H14C	109.5
C4—C5—Br1	119.1 (5)	H14A—C14—H14C	109.5
C6—C5—Br1	119.7 (5)	H14B—C14—H14C	109.5
C7—C6—C5	119.3 (6)	N2—C15—H15A	109.5
C7—C6—Br2	120.4 (5)	N2—C15—H15B	109.5
C5—C6—Br2	120.2 (6)	H15A—C15—H15B	109.5
C8—C7—C6	119.7 (6)	N2—C15—H15C	109.5
C8—C7—Br3	120.0 (6)	H15A—C15—H15C	109.5
C6—C7—Br3	120.3 (5)	H15B—C15—H15C	109.5
C7—C8—C3	121.4 (6)		

C9—O1—C1—O2	0.1 (10)	C4—C5—C6—Br2	179.9 (5)
C9—O1—C1—C3	−179.8 (6)	Br1—C5—C6—Br2	−3.4 (7)
O2—C1—C3—C8	−106.3 (8)	C5—C6—C7—C8	−4.5 (10)
O1—C1—C3—C8	73.6 (8)	Br2—C6—C7—C8	177.6 (5)
O2—C1—C3—C4	75.4 (9)	C5—C6—C7—Br3	175.3 (5)
O1—C1—C3—C4	−104.8 (7)	Br2—C6—C7—Br3	−2.6 (8)
C8—C3—C4—C5	−1.0 (9)	C6—C7—C8—C3	4.3 (10)
C1—C3—C4—C5	177.4 (6)	Br3—C7—C8—C3	−175.5 (5)
C8—C3—C4—C2	174.8 (6)	C6—C7—C8—Br4	−178.6 (5)
C1—C3—C4—C2	−6.9 (9)	Br3—C7—C8—Br4	1.5 (7)
O4—C2—C4—C5	61.8 (9)	C4—C3—C8—C7	−1.5 (9)
O3—C2—C4—C5	−118.4 (7)	C1—C3—C8—C7	−179.9 (6)
O4—C2—C4—C3	−113.8 (7)	C4—C3—C8—Br4	−178.7 (4)
O3—C2—C4—C3	65.9 (9)	C1—C3—C8—Br4	3.0 (8)
C3—C4—C5—C6	0.8 (9)	C10′—N1—C10—C11	40 (10)
C2—C4—C5—C6	−174.8 (6)	N1—C10—C11—C12	176 (2)
C3—C4—C5—Br1	−175.9 (4)	C10—N1—C10′—C11′	−47 (9)
C2—C4—C5—Br1	8.6 (8)	N1—C10′—C11′—C12′	−141 (4)
C4—C5—C6—C7	2.0 (9)	C14—N2—C13—O5	−0.5 (13)
Br1—C5—C6—C7	178.6 (5)	C15—N2—C13—O5	179.4 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O3	0.89	1.87	2.757 (7)	175
N1—H1*B*···O4^{i}	0.89	2.04	2.812 (8)	144
N1—H1*C*···O5^{ii}	0.89	1.91	2.762 (8)	160

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+1/2; (ii) *x*, *y*−1, *z*.