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Methyl [(3,4,5-tribromo-1*H*-pyrrolyl-2-carbonyl)amino]acetate 0.25-hydrate

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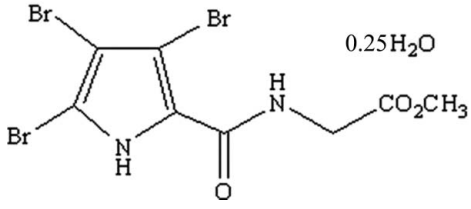
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.010 Å; R factor = 0.043; wR factor = 0.099; data-to-parameter ratio = 16.4.

The asymmetric unit of the title compound, $C_8H_7Br_3N_2O_3\cdot 0.25H_2O$, consists of two organic molecules, one water O atom and an attached H atom; the water O atom lies on a crystallographic twofold rotation axis. Intermolecular N—H···O hydrogen-bond interactions link molecules of the organic compound (the acetate), forming dimers. These dimers are linked by O(W)—H(W)···O and N—H···O(W) hydrogen bonds, generating a three-dimensional network.

Related literature

For related literature, see: Banwell *et al.* (2006); Bernstein *et al.* (1995); Faulkner (2002); Sosa *et al.* (2002); Zeng (2006); Zeng *et al.* (2006).



Experimental

Crystal data

$C_8H_7Br_3N_2O_3\cdot 0.25H_2O$
M_r = 423.39
Monoclinic, $P2/n$
a = 15.9656 (19) Å
b = 9.7566 (12) Å
c = 16.1805 (19) Å
β = 102.625 (2)°
V = 2459.5 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 9.84 mm^{-1}
T = 293 (2) K
0.41 × 0.29 × 0.24 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.107, T_{max} = 0.201
(expected range = 0.050–0.094)
14610 measured reflections
4828 independent reflections
2608 reflections with $I > 2\sigma(I)$
R_{int} = 0.076

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.099
S = 1.01
4828 reflections
294 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O7	0.86	2.53	3.202 (8)	136
O7—H7···O2^{i}	0.85	2.02	2.866 (6)	180
N3—H3···O4^{ii}	0.86	1.91	2.756 (8)	167
N1—H1···O1^{iii}	0.86	1.92	2.772 (8)	168

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

Data collection: *SMART* (Bruker,1999); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: HG2225).

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supplementary materials

Acta Cryst. (2007). E**63**, o2712 [**doi:10.1107/S1600536807019289**]

Methyl [(3,4,5-tribromo-1*H*-pyrrolyl-2-carbonyl)amino]acetate 0.25-hydrate

X.-C. Zeng, X.-L. Xu, X. Ling, J. Zeng and X. Li

Comment

Pyrrole derivatives are well-known in many marine organisms (Faulkner, 2002), some show important bioactivities, such as antitumor activity (Banwell *et al.*, 2006) and protein kinase inhibiting activity (Sosa *et al.*, 2002). This is the reason why they have attracted our interest. This study follows our previous studies on 3-[(3,4,5-Tribromo-1*H*-pyrrol-2-ylcarbonyl)amino]propanoic acid (Zeng *et al.*, 2006) and 3-Bromo-1-methyl-6,7-dihydropyrrolo[2,3-c]azepine-4,8(1*H*,5H)-dione (Zeng, 2006).

In the crystal structure, there are 8 molecules of Methyl [(3,4,5-tribromo-1*H*-pyrrole-2-carbonyl)amino]acetate and 2 crystal water molecules in each unit cell. Molecules of the acetate are linked through N—H···O H-bonds (Table 1) to form centrosymmetric dimers (Fig. 2) of graph-set motif $R_2^2(10)$ (Bernstein *et al.*, 1995). These dimers are connected by O—H(W)···O and N—H···O(W) H-bond interactions, generating the 3D network (Fig. 3). Bond lengths and angles are unexceptional.

Experimental

The hydrochloride of glycine methyl ester (0.63 g, 5 mmol) and 3,4,5-tribromo-2-trichloroacetylpyrrole (2.25 g, 5 mmol) were added to acetonitrile (12 ml), followed by the dropwise addition of triethylamine (1.4 ml). The mixture was stirred at room temperature for 16 h and then poured into water. After filtration, the precipitate was collected as a yellow solid. The impure product was dissolved in 95% EtOH at room temperature. Colourless monoclinic crystals suitable for X-ray analysis (m.p. 470 K, 87.6% yield) grew over a period of one week when the solution was exposed to the air. CH&N elemental analysis. Calc. for $C_8H_{7.5}Br_3N_2O_{3.25}$: C 22.70, H 1.79, N 6.62%; found: C 22.65, H 1.83, N 6.68%.

Refinement

All non-H atoms were refined with anisotropic displacement parameters. All H atoms except the H(W) were positioned geometrically [C—H = 0.97Å for CH_2, 0.96Å for CH_3, and N—H = 0.86 Å] and refined using a riding model, with U_{iso} = 1.2U_{eq} (1.5U_{eq} for the methyl group) of the parent atom. The H atoms attached to water O atoms in the difference Fourier maps were constrained to their parent O atoms with distance of O—H = 0.8498, and with U_{iso} = 1.5U_{eq}.

Figures

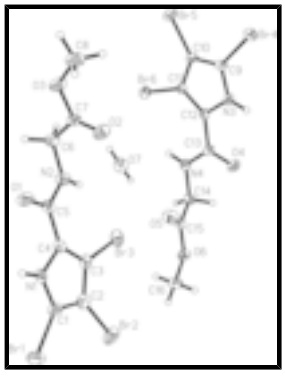

Fig. 1. The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

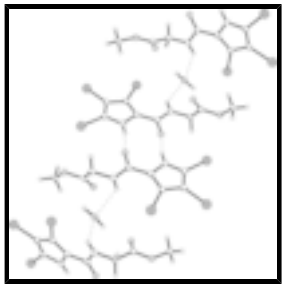

Fig. 2. Dimers & chain formed by hydrogen bonds (dashed lines).

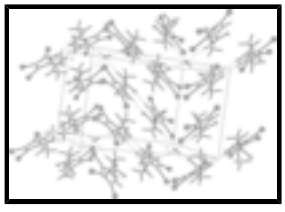

Fig. 3. Crystal packing of compound I and crystal water showing the 3D network formed by hydrogen bonds (dashed lines).

(I)

Crystal data

$C_8H_7Br_3N_2O_3·0.25H_2O$	F_{000} = 1604
M_r = 423.39	D_x = 2.287 Mg m^{-3}
Monoclinic, *P*2/*n*	Melting point: 470 K
Hall symbol: -P 2yac	Mo *K*α radiation λ = 0.71073 Å
a = 15.9656 (19) Å	Cell parameters from 2696 reflections
b = 9.7566 (12) Å	θ = 2.6–22.7º
c = 16.1805 (19) Å	μ = 9.84 mm^{-1}
β = 102.625 (2)º	*T* = 293 (2) K
V = 2459.5 (5) Å^3	Prism, colourless
Z = 8	0.41 × 0.29 × 0.24 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer	4828 independent reflections

Radiation source: fine-focus sealed tube
Monochromator: graphite
T = 293(2) K
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.107, T_{max} = 0.201
14610 measured reflections
2608 reflections with $I > 2\sigma(I)$
R_{int} = 0.076
θ_{max} = 26.0º
θ_{min} = 1.6º
h = −19→19
k = −12→11
l = −19→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.099
S = 1.01
4828 reflections
294 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 4.7343P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}
Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br6	0.28459 (5)	0.85330 (8)	0.06071 (5)	0.0418 (2)
Br4	0.14598 (5)	0.44478 (9)	−0.19238 (5)	0.0432 (2)
Br3	0.23755 (5)	0.37740 (9)	0.37613 (5)	0.0495 (3)
Br5	0.32222 (5)	0.68636 (9)	−0.12494 (5)	0.0496 (3)
Br1	0.32381 (6)	0.02225 (10)	0.66869 (5)	0.0600 (3)
Br2	0.16429 (6)	0.26370 (10)	0.55774 (7)	0.0649 (3)
O6	0.0297 (3)	0.6921 (5)	0.3266 (3)	0.0418 (13)
N1	0.3844 (4)	0.0974 (6)	0.5250 (4)	0.0356 (16)

H1	0.4275	0.0429	0.5392	0.043*
C9	0.1664 (5)	0.5607 (7)	−0.0988 (4)	0.0316 (18)
N3	0.1121 (4)	0.5678 (6)	−0.0457 (3)	0.0328 (15)
H3	0.0665	0.5191	−0.0499	0.039*
N2	0.4197 (4)	0.2645 (6)	0.3347 (4)	0.0416 (17)
H2	0.3780	0.3223	0.3267	0.050*
O4	0.0220 (3)	0.6163 (6)	0.0733 (3)	0.0484 (15)
C13	0.0894 (5)	0.6823 (8)	0.0805 (5)	0.0301 (17)
C5	0.4292 (5)	0.1736 (8)	0.3990 (4)	0.0361 (19)
O2	0.3963 (3)	0.0869 (6)	0.1948 (3)	0.0492 (15)
C4	0.3680 (5)	0.1792 (7)	0.4544 (4)	0.0291 (17)
O1	0.4869 (3)	0.0887 (6)	0.4100 (3)	0.0503 (15)
C12	0.1402 (4)	0.6641 (7)	0.0160 (4)	0.0285 (17)
O5	0.1188 (4)	0.5676 (6)	0.2663 (3)	0.0551 (16)
O3	0.5235 (3)	0.1515 (5)	0.1720 (3)	0.0519 (16)
C15	0.0769 (5)	0.6658 (9)	0.2688 (4)	0.0358 (19)
C2	0.2633 (5)	0.2076 (8)	0.5261 (5)	0.038 (2)
C11	0.2156 (4)	0.7166 (7)	−0.0008 (4)	0.0285 (17)
N4	0.1166 (4)	0.7679 (6)	0.1437 (4)	0.0346 (15)
H4	0.1635	0.8131	0.1469	0.041*
C7	0.4587 (5)	0.1569 (8)	0.2114 (5)	0.0325 (19)
C1	0.3226 (5)	0.1157 (8)	0.5684 (5)	0.040 (2)
C10	0.2308 (4)	0.6520 (7)	−0.0732 (4)	0.0320 (18)
C16	0.0345 (6)	0.5903 (9)	0.3918 (5)	0.060 (3)
H16A	−0.0080	0.5208	0.3729	0.089*
H16B	0.0241	0.6327	0.4422	0.089*
H16C	0.0905	0.5494	0.4039	0.089*
C3	0.2933 (5)	0.2478 (7)	0.4538 (5)	0.0325 (18)
C8	0.5159 (6)	0.0477 (9)	0.1066 (5)	0.066 (3)
H8A	0.5081	−0.0404	0.1303	0.100*
H8B	0.5671	0.0468	0.0847	0.100*
H8C	0.4674	0.0680	0.0617	0.100*
C14	0.0669 (5)	0.7852 (7)	0.2076 (4)	0.0358 (19)
H14A	0.0068	0.7949	0.1802	0.043*
H14B	0.0848	0.8687	0.2390	0.043*
C6	0.4787 (5)	0.2648 (8)	0.2798 (5)	0.040 (2)
H6A	0.5362	0.2496	0.3133	0.048*
H6B	0.4777	0.3543	0.2535	0.048*
O7	0.2500	0.9820 (8)	0.2500	0.059 (2)*
H7	0.2933	1.0136	0.2337	0.37 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br6	0.0355 (5)	0.0446 (5)	0.0444 (5)	−0.0109 (4)	0.0070 (4)	−0.0039 (4)
Br4	0.0459 (5)	0.0500 (6)	0.0341 (4)	−0.0044 (4)	0.0096 (4)	−0.0073 (4)
Br3	0.0435 (5)	0.0444 (5)	0.0548 (6)	0.0136 (4)	−0.0017 (4)	−0.0009 (4)
Br5	0.0408 (5)	0.0637 (6)	0.0507 (5)	−0.0116 (5)	0.0236 (4)	−0.0056 (5)

Br1	0.0650 (6)	0.0739 (7)	0.0470 (5)	0.0008 (5)	0.0255 (5)	0.0096 (5)
Br2	0.0386 (5)	0.0773 (7)	0.0843 (7)	0.0076 (5)	0.0258 (5)	−0.0145 (6)
O6	0.036 (3)	0.052 (4)	0.042 (3)	0.004 (3)	0.018 (3)	0.000 (3)
N1	0.030 (4)	0.042 (4)	0.033 (4)	0.015 (3)	0.002 (3)	0.006 (3)
C9	0.039 (5)	0.030 (5)	0.028 (4)	0.004 (4)	0.013 (4)	0.001 (3)
N3	0.026 (3)	0.036 (4)	0.036 (4)	−0.007 (3)	0.007 (3)	0.003 (3)
N2	0.046 (4)	0.041 (4)	0.042 (4)	0.014 (3)	0.018 (3)	0.003 (3)
O4	0.036 (3)	0.063 (4)	0.052 (3)	−0.021 (3)	0.021 (3)	−0.019 (3)
C13	0.023 (4)	0.033 (5)	0.036 (4)	0.001 (4)	0.011 (4)	0.000 (4)
C5	0.041 (5)	0.040 (5)	0.027 (4)	−0.001 (4)	0.007 (4)	−0.002 (4)
O2	0.045 (4)	0.043 (4)	0.063 (4)	−0.011 (3)	0.020 (3)	−0.002 (3)
C4	0.033 (4)	0.023 (4)	0.030 (4)	0.004 (4)	0.004 (4)	−0.003 (3)
O1	0.042 (3)	0.061 (4)	0.055 (4)	0.030 (3)	0.026 (3)	0.018 (3)
C12	0.023 (4)	0.031 (5)	0.029 (4)	−0.002 (3)	0.001 (3)	0.002 (4)
O5	0.065 (4)	0.052 (4)	0.052 (4)	0.027 (3)	0.020 (3)	0.007 (3)
O3	0.051 (4)	0.057 (4)	0.056 (4)	−0.021 (3)	0.029 (3)	−0.019 (3)
C15	0.032 (5)	0.049 (6)	0.027 (4)	−0.001 (4)	0.008 (4)	−0.006 (4)
C2	0.037 (5)	0.034 (5)	0.042 (5)	0.001 (4)	0.010 (4)	−0.021 (4)
C11	0.029 (4)	0.031 (4)	0.025 (4)	−0.010 (4)	0.005 (3)	0.003 (3)
N4	0.034 (4)	0.036 (4)	0.035 (4)	−0.014 (3)	0.011 (3)	−0.013 (3)
C7	0.034 (5)	0.031 (5)	0.034 (5)	0.003 (4)	0.012 (4)	0.010 (4)
C1	0.037 (5)	0.047 (5)	0.039 (5)	0.001 (4)	0.017 (4)	−0.007 (4)
C10	0.029 (4)	0.040 (5)	0.031 (4)	−0.005 (4)	0.014 (4)	−0.003 (4)
C16	0.066 (6)	0.081 (7)	0.038 (5)	−0.008 (5)	0.024 (5)	0.005 (5)
C3	0.029 (4)	0.025 (4)	0.041 (5)	0.005 (4)	0.002 (4)	−0.007 (4)
C8	0.067 (6)	0.084 (7)	0.057 (6)	−0.020 (6)	0.033 (5)	−0.033 (5)
C14	0.040 (5)	0.037 (5)	0.033 (4)	0.002 (4)	0.013 (4)	−0.011 (4)
C6	0.047 (5)	0.038 (5)	0.038 (5)	−0.002 (4)	0.017 (4)	0.004 (4)

Geometric parameters (Å, °)

Br6—C11	1.872 (7)	C4—C3	1.367 (9)
Br4—C9	1.861 (7)	C12—C11	1.388 (9)
Br3—C3	1.866 (7)	O5—C15	1.174 (8)
Br5—C10	1.865 (7)	O3—C7	1.331 (8)
Br1—C1	1.857 (8)	O3—C8	1.450 (8)
Br2—C2	1.847 (7)	C15—C14	1.514 (10)
O6—C15	1.348 (8)	C2—C1	1.373 (10)
O6—C16	1.439 (9)	C2—C3	1.413 (10)
N1—C1	1.342 (8)	C11—C10	1.398 (9)
N1—C4	1.371 (8)	N4—C14	1.444 (8)
N1—H1	0.8600	N4—H4	0.8600
C9—N3	1.349 (8)	C7—C6	1.511 (10)
C9—C10	1.355 (9)	C16—H16A	0.9600
N3—C12	1.373 (8)	C16—H16B	0.9600
N3—H3	0.8600	C16—H16C	0.9600
N2—C5	1.350 (9)	C8—H8A	0.9600
N2—C6	1.429 (8)	C8—H8B	0.9600
N2—H2	0.8600	C8—H8C	0.9600

O4—C13	1.237 (8)	C14—H14A	0.9700
C13—N4	1.319 (8)	C14—H14B	0.9700
C13—C12	1.466 (9)	C6—H6A	0.9700
C5—O1	1.223 (8)	C6—H6B	0.9700
C5—C4	1.463 (9)	O7—H7	0.8498
O2—C7	1.189 (8)		
C15—O6—C16	115.5 (6)	C14—N4—H4	120.4
C1—N1—C4	109.3 (6)	O2—C7—O3	124.8 (7)
C1—N1—H1	125.3	O2—C7—C6	126.7 (7)
C4—N1—H1	125.3	O3—C7—C6	108.5 (6)
N3—C9—C10	108.8 (6)	N1—C1—C2	109.4 (7)
N3—C9—Br4	121.8 (6)	N1—C1—Br1	121.6 (6)
C10—C9—Br4	129.4 (5)	C2—C1—Br1	129.1 (6)
C9—N3—C12	110.2 (6)	C9—C10—C11	107.0 (6)
C9—N3—H3	124.9	C9—C10—Br5	126.7 (5)
C12—N3—H3	124.9	C11—C10—Br5	126.3 (6)
C5—N2—C6	120.1 (6)	O6—C16—H16A	109.5
C5—N2—H2	119.9	O6—C16—H16B	109.5
C6—N2—H2	119.9	H16A—C16—H16B	109.5
O4—C13—N4	122.4 (7)	O6—C16—H16C	109.5
O4—C13—C12	118.4 (7)	H16A—C16—H16C	109.5
N4—C13—C12	119.3 (6)	H16B—C16—H16C	109.5
O1—C5—N2	120.7 (7)	C4—C3—C2	108.2 (7)
O1—C5—C4	121.2 (7)	C4—C3—Br3	128.5 (6)
N2—C5—C4	118.0 (7)	C2—C3—Br3	123.2 (6)
C3—C4—N1	107.3 (6)	O3—C8—H8A	109.5
C3—C4—C5	135.5 (7)	O3—C8—H8B	109.5
N1—C4—C5	117.2 (6)	H8A—C8—H8B	109.5
N3—C12—C11	105.6 (6)	O3—C8—H8C	109.5
N3—C12—C13	117.2 (6)	H8A—C8—H8C	109.5
C11—C12—C13	137.1 (7)	H8B—C8—H8C	109.5
C7—O3—C8	115.3 (6)	N4—C14—C15	112.5 (6)
O5—C15—O6	126.0 (7)	N4—C14—H14A	109.1
O5—C15—C14	125.8 (7)	C15—C14—H14A	109.1
O6—C15—C14	108.2 (7)	N4—C14—H14B	109.1
C1—C2—C3	105.8 (6)	C15—C14—H14B	109.1
C1—C2—Br2	126.4 (6)	H14A—C14—H14B	107.8
C3—C2—Br2	127.8 (6)	N2—C6—C7	113.0 (6)
C12—C11—C10	108.4 (6)	N2—C6—H6A	109.0
C12—C11—Br6	126.4 (5)	C7—C6—H6A	109.0
C10—C11—Br6	125.2 (5)	N2—C6—H6B	109.0
C13—N4—C14	119.3 (6)	C7—C6—H6B	109.0
C13—N4—H4	120.4	H6A—C6—H6B	107.8
C10—C9—N3—C12	−0.1 (8)	C4—N1—C1—Br1	−179.5 (5)
Br4—C9—N3—C12	−177.8 (5)	C3—C2—C1—N1	−1.2 (9)
C6—N2—C5—O1	−1.7 (11)	Br2—C2—C1—N1	178.1 (5)
C6—N2—C5—C4	178.8 (6)	C3—C2—C1—Br1	179.9 (6)
C1—N1—C4—C3	−1.0 (8)	Br2—C2—C1—Br1	−0.8 (11)

C1—N1—C4—C5	179.7 (6)	N3—C9—C10—C11	0.6 (8)
O1—C5—C4—C3	−171.0 (8)	Br4—C9—C10—C11	178.1 (5)
N2—C5—C4—C3	8.5 (13)	N3—C9—C10—Br5	−179.0 (5)
O1—C5—C4—N1	7.9 (11)	Br4—C9—C10—Br5	−1.5 (11)
N2—C5—C4—N1	−172.6 (6)	C12—C11—C10—C9	−0.9 (8)
C9—N3—C12—C11	−0.5 (8)	Br6—C11—C10—C9	−179.6 (5)
C9—N3—C12—C13	−178.5 (6)	C12—C11—C10—Br5	178.7 (5)
O4—C13—C12—N3	−4.0 (10)	Br6—C11—C10—Br5	0.0 (10)
N4—C13—C12—N3	176.1 (6)	N1—C4—C3—C2	0.3 (8)
O4—C13—C12—C11	178.8 (8)	C5—C4—C3—C2	179.3 (8)
N4—C13—C12—C11	−1.1 (13)	N1—C4—C3—Br3	178.5 (5)
C16—O6—C15—O5	1.9 (11)	C5—C4—C3—Br3	−2.5 (13)
C16—O6—C15—C14	−177.9 (6)	C1—C2—C3—C4	0.5 (8)
N3—C12—C11—C10	0.8 (8)	Br2—C2—C3—C4	−178.8 (5)
C13—C12—C11—C10	178.2 (8)	C1—C2—C3—Br3	−177.8 (5)
N3—C12—C11—Br6	179.5 (5)	Br2—C2—C3—Br3	2.9 (10)
C13—C12—C11—Br6	−3.1 (13)	C13—N4—C14—C15	75.8 (8)
O4—C13—N4—C14	0.5 (11)	O5—C15—C14—N4	−0.9 (11)
C12—C13—N4—C14	−179.6 (6)	O6—C15—C14—N4	178.9 (6)
C8—O3—C7—O2	−2.3 (11)	C5—N2—C6—C7	81.4 (9)
C8—O3—C7—C6	177.3 (6)	O2—C7—C6—N2	8.7 (11)
C4—N1—C1—C2	1.4 (9)	O3—C7—C6—N2	−170.9 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O7	0.86	2.53	3.202 (8)	136
O7—H7···O2^{i}	0.85	2.02	2.866 (6)	180
N3—H3···O4^{ii}	0.86	1.91	2.756 (8)	167
N1—H1···O1^{iii}	0.86	1.92	2.772 (8)	168

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

Fig. 1

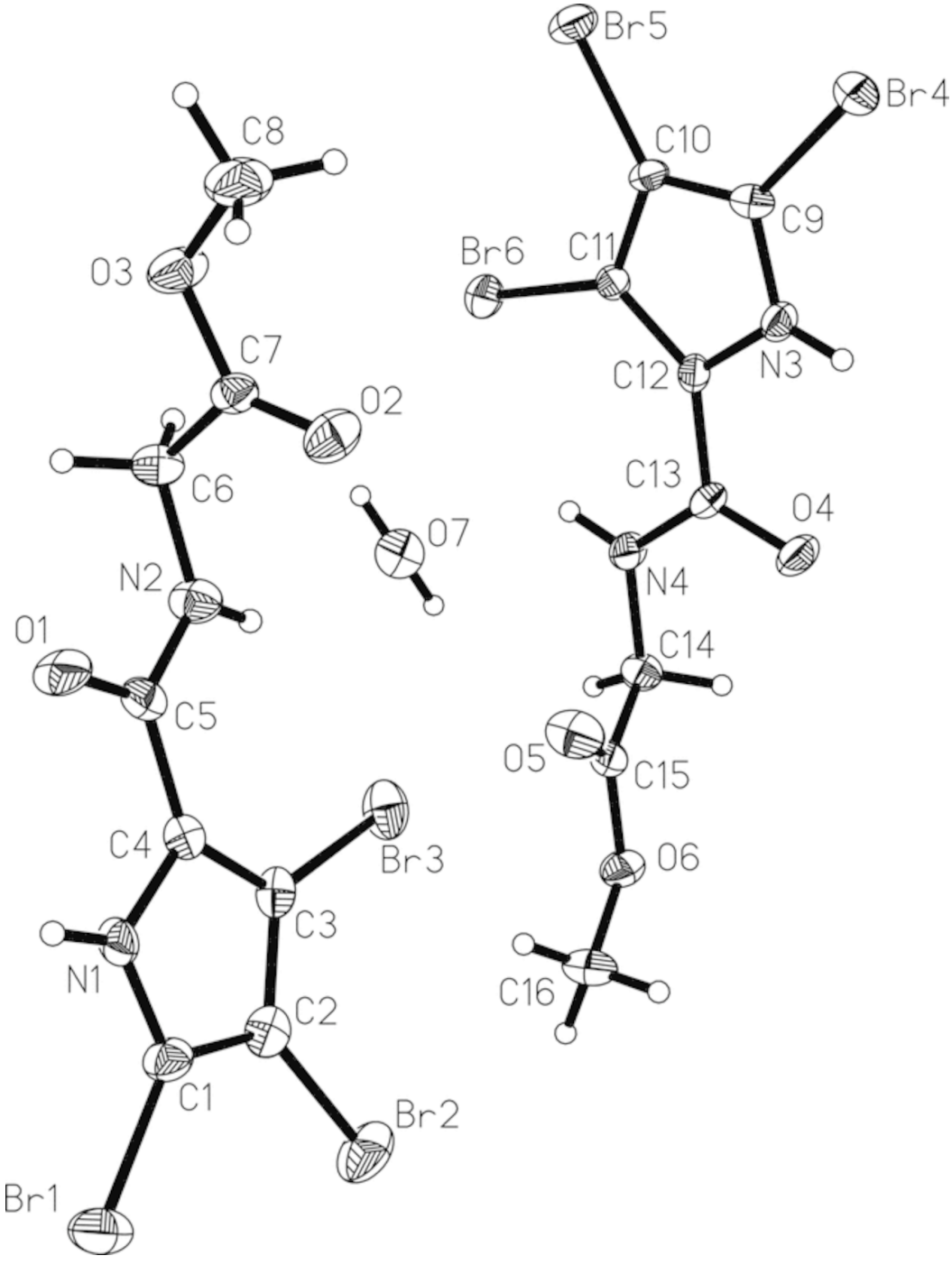
Br5
Br4
C8
C10
C9
Br6
C11
O3
C7
C12
N3
O2
C13
C6
O4
O7
N2
N4
O1
C14
C5
O5
C15
C4
Br3
O6
C3
N1
C16
C2
C1
Br2
Br1

Fig. 2

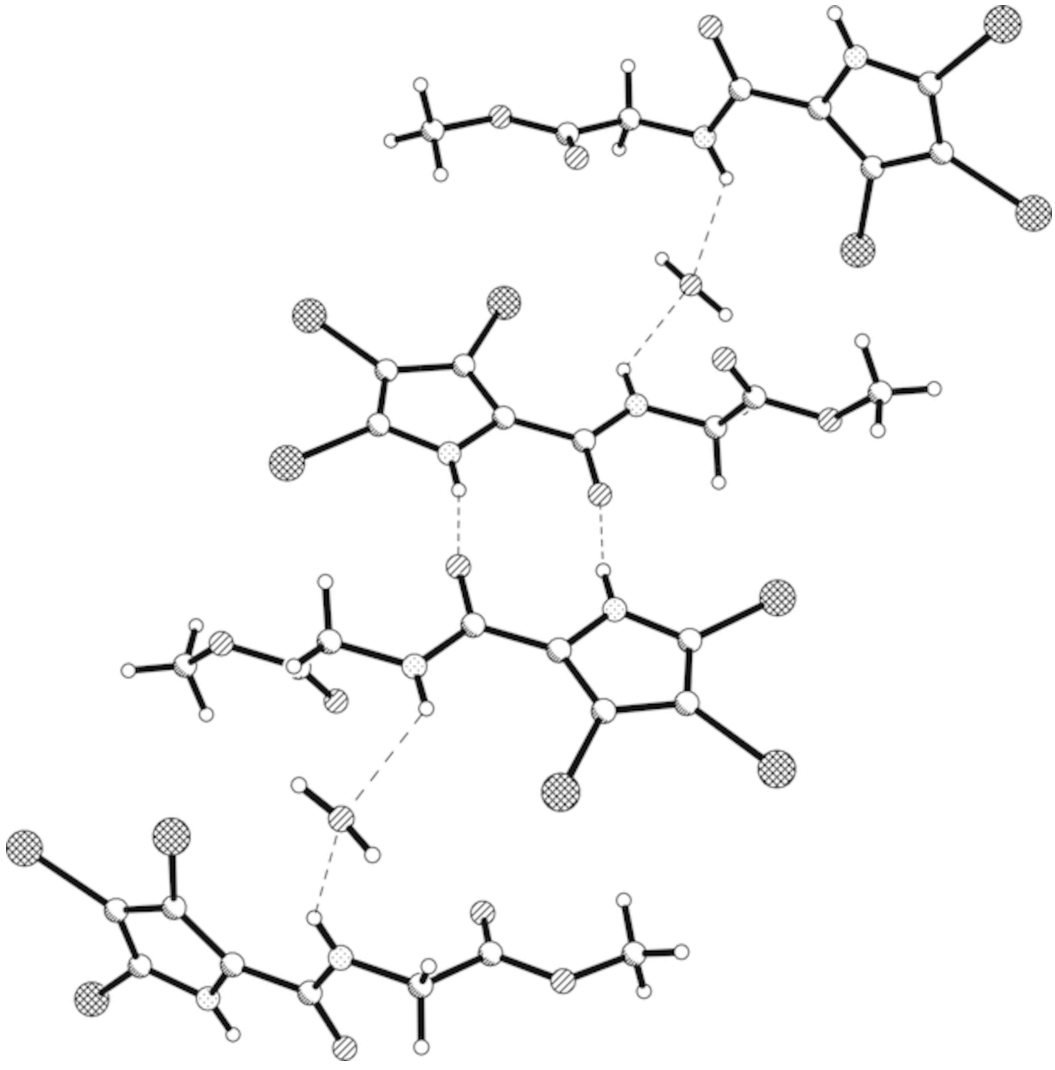

Fig. 3