research communications

Synthesis and crystal structure of a new pyridinium bromide salt: 4-methyl-1-(3-phenoxypropyl)-pyridinium bromide

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In the cation of the title molecular salt, $C_{15}H_{18}NO^+ \cdot Br^-$, the pyridinium and phenyl rings are inclined to one another by 11.80 (8)°. In the crystal, the Br^- anion is linked to the cation by a C—H···Br hydrogen bond. The cations stack along the b-axis direction and are linked by further C—H···Br interactions, and offset π–π interactions [intercentroid distances = 3.5733 (19) and 3.8457 (19) Å], forming slabs parallel to the ab plane. The effects of the C—H···X^- interaction on the NMR signals of the ortho- and meta-pyridinium protons in a series of related ionic liquids, viz. 4-methyl-1-(4-phenoxybutyl)pyridin-1-ium salts, are reported and discussed.

1. Chemical context

In the last two decades, ionic liquids (ILs) have gained considerable interest as excellent alternatives to volatile organic compounds (VOCs) because of their unusual range of properties such as negligible vapour pressure, excellent thermal stability in a wide temperature range, no flammability, high ionic conductivity and solvation ability (Davis, 2004).

A wide range of applications using ionic liquids has been reported in many areas such as solvents in organic synthesis (Wang et al., 2007), media for electrodeposition of metals (Endres, 2002), corrosion inhibitors (Ibrahim et al., 2011), electrolytes for electrochemical devices such as batteries (Brennecke & Maginn, 2001), catalysts (Shi et al. 2004), in fuel cells (De Souza et al., 2006), in polymer science (Kubisa, 2004), and in dye-sensitized solar cells (Kawano et al., 2004).

In view of the above mentioned, and of our ongoing research interest in the synthesis of ionic liquids (Messali, 2016, 2015; Messali et al., 2014), we present in this study the preparation and the crystal structure of the novel title pyridinium halide salt, 4-methyl-1-(3-phenoxypropyl)pyridinium bromide.
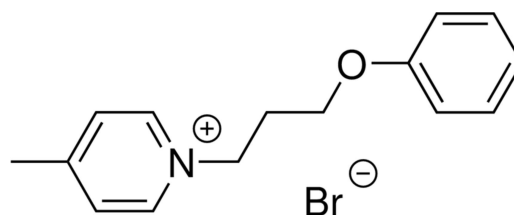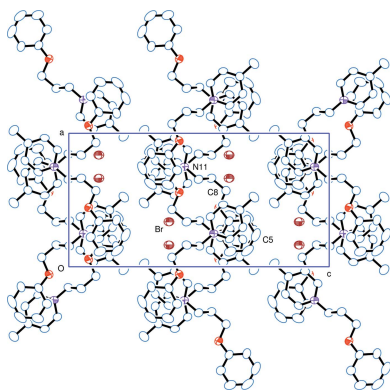
Table 1
Hydrogen-bond geometry (Å, °).

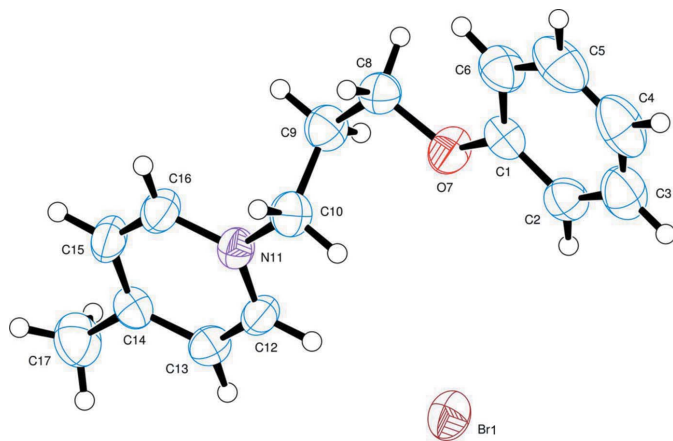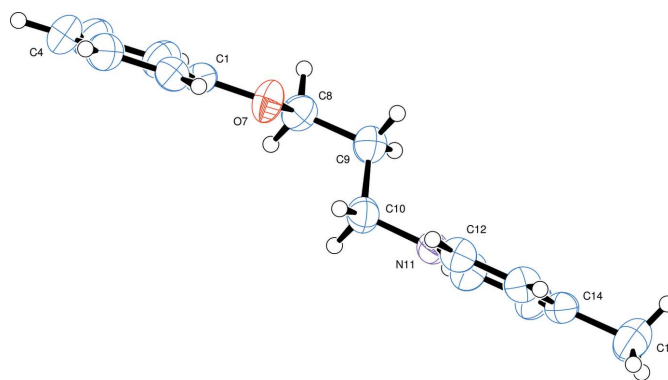| $D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C10—H10A···O7	0.97	2.52	2.850 (3)	100
C10—H10B···Br1^i	0.97	2.89	3.735 (3)	146
C10—H10A···Br1	0.97	3.11	4.043 (3)	163
C12—H12···Br1	0.93	3.08	3.940 (3)	154
C15—H15···Br1^{ii}	0.93	3.07	3.931 (3)	155
C17—H17B···Br1^{ii}	0.96	3.08	3.956 (4)	152

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (ii) $x + 1, y, z$.

2. Structural commentary

The molecular structure of the title pyridinium bromide salt is illustrated in Fig. 1. There is a weak intramolecular C—H···O contact present, with an H···O distance of 2.52 Å and a C—H···O angle of only 100° (see Table 1). The cation consists of two planar groups, a pyridinium ring (N11/C12–C16) and a phenyl group (C1–C6); atom N11 has the expected planar–trigonal conformation. The two aromatic rings are inclined to one another by 11.80 (8)° and there is a step of *ca* 1.35 Å between the two groups along the C9—C10 bond, see Fig. 2. The C1—O7, C8—C9, C10—N11 and C14—C17 bonds are roughly parallel, so that the two aromatic groups are at opposite ends of an approximately linear cation. This is in contrast to the alignment found in 1-[2-(5-nitro-1*H*-indol-2-yl)phenyl]methylpyridinium chloride where the cation is U-shaped with the pyridinium ring lying over the pyrrolo ring of the indole moiety (Bremner *et al.*, 2011), possibly as a result of electronic interactions between the two rings.

3. Supramolecular features

In the crystal, the bromide anion is linked to the cation by a C10—H10B···Br1^i hydrogen bond (Table 1). The anion is surrounded by three other cations with the most significant C-–H···Br short contacts varying from *ca* 3.07 to 3.11 Å (Table 1). The bromide ions are aligned approximately in the

Figure 2
A view of the cation showing the step formation about bond C9—C10 and the approximately parallel ring planes.

planes of the aromatic rings, which is similar to the arrangement found in *N*-benzylpyridinium bromide (Anders *et al.*, 1990), and in contrast to those in a series of *N*-(pentafluoro-benzyl)pyridinium salts where the anion faces the aromatic rings with formation of anion–π interactions (Giese *et al.*, 2014).

The cations stack head-to-tail, in pairs about centres of symmetry, along the *b*-axis direction with the aromatic rings being inclined slightly to one another [α = 11.80 (8)° within a pair and 7.52 (16)° between pairs]. As shown in Fig. 3, the pairs are linked by offset π–π interactions, forming slabs parallel to (001): *Cg*1···*Cg*2^{iii} = 3.8457 (19) Å within a pair, and *Cg*1···*Cg*2^{iv} = 3.5733 (19) Å between pairs; *Cg*1 and *Cg*2 are the centroids of rings C1—C6 and N11/C12–C16, respectively; symmetry codes: (iii) $1 - x, 1 - y, 1 - z$; (iv) $x - \frac{1}{2}, \frac{3}{2} - y, 1 - z$.

Figure 1
The molecular structure of the component ions of the title salt, indicating the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.
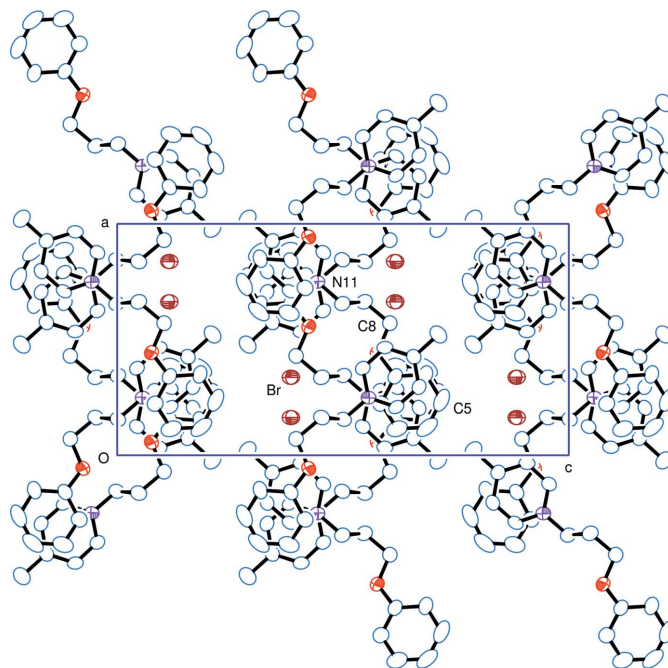

Figure 3
Crystal packing viewed along the *b* axis, showing the stacking of the phenyl and pyridinium groups along that axis.

Table 2
^{1}H NMR chemical shifts (D$_2$O, δ p.p.m.) for the pyridinium hydrogen atoms (Ha and Hb) of a series of ionic liquids (1–7)* and the title salt.

| Ionic liquid	Anion	Chemical shift for Ha	Chemical shift for Hb
1	Br$^-$	d, 9.23	d, 7.67
2	NO$_3^-$	d, 9.22	d, 7.66
3	CF$_3$CO$_2^-$	d, 9.09	d, 7.65
4	PF$_6^-$	d, 8.94	d, 7.94
5	SCN$^-$	d, 8.82	d, 7.80
6	N(CN)$_2^-$	d, 8.91	d, 7.75
7	BF$_4^-$	d, 8.60	d, 7.69
This study	Br$^-$	d, 8.48	d, 7.66

*Messali (2015).

4. C—H⋯anion interactions in the ^{1}H NMR spectrum

The C—H⋯anion interactions are clearly manifested in the ^{1}H NMR spectrum (see Section 5. *Synthesis and crystallization*). Such an effect has previously been shown by a solution study of the C—H⋯Br interaction on the signals of the *ortho*- and *meta*-pyridinium protons in the ^{1}H NMR spectra of a series of *N*-(pentafluorobenzyl)pyridinium salts (Giese *et al.*, 2014). The present study in D$_2$O solvent involves only the pyridinium protons (Ha and Hb) of a series of 4-methyl-1-(4-phenoxybutyl)pyridin-1-ium X^- ionic liquids, and the title compound, shown in Fig. 4. The results, given in Table 2, reveal significant shifts for the hydrogen atom Ha in various pyridinium salts, whereas hydrogen atom Hb is only slightly affected by the different counter-anions (Messali, 2015); *viz.* the study reveals a range of 0.75 p.p.m. for the signals of the *ortho*-pyridinium protons (Ha) and a shorter range of 0.29 p.p.m. for *meta*-pyridinium protons (Hb). The determination of the causes behind this variation remains a challenging task for our research group.

5. Synthesis and crystallization

The synthesis of the title compound is illustrated in Fig. 5. To a solution of 1 g of 4-picoline (10.7 mmol) in 20 ml of toluene, were added 2.53 g of (3-bromopropoxy)benzene (118 mmol) at room temperature, followed by stirring at 355 K for 18 h.
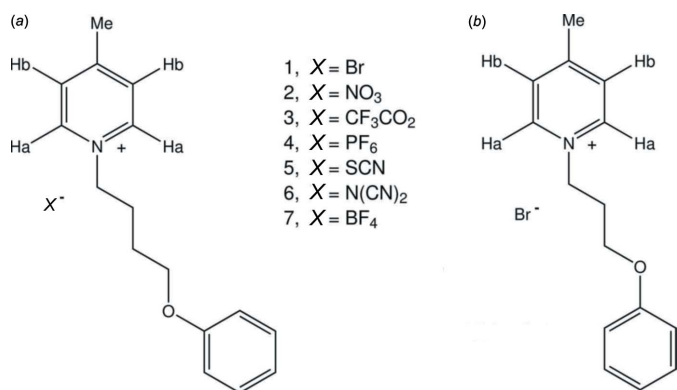
Figure 4
A series of ionic liquids: (*a*) 4-methyl-1-(4-phenoxybutyl)pyridin-1-ium salts with various counter-anions; (*b*) this study: 4-methyl-1-(3-phenoxypropyl)pyridinium bromide.
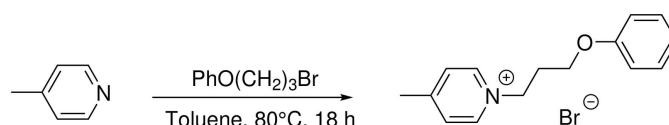
Table 3
Experimental details.

Crystal data	
Chemical formula	C$_{15}$H$_{18}$NO$^+$·Br$^-$
M_r	308.21
Crystal system, space group	Orthorhombic, $Pbca$
Temperature (K)	295
a, b, c (Å)	10.3615 (3), 13.8916 (6), 20.2121 (8)
V (Å^3)	2909.29 (19)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.82
Crystal size (mm)	0.60 × 0.19 × 0.10
Data collection	
Diffractometer	Oxford Diffraction Xcalibur 3/ Sapphire3 CCD
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.529, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38980, 2560, 2212
R_{int}	0.048
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.087, 1.20
No. of reflections	2560
No. of parameters	164
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.27, −0.25

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012).

The completion of the reaction was marked by the separation of a solid from the initially obtained clear and homogeneous mixture of the starting materials. The product was isolated by filtration to remove the unreacted starting materials and solvent. Subsequently, the title picolinium salt was washed with ethyl acetate. The product was finally dried at reduced pressure to remove all volatile organic compounds. The title compound was obtained as a white solid. Colourless prismatic crystals were obtained by slow evaporation of a solution in dichloromethane.

Spectroscopic and analytical data: ^{1}H NMR (D$_2$O, 400 MHz): δ = 2.34 (*quint*, J = 7.6 Hz, 2H), 2.50 (*s*, 3H), 3.98 (*t*, J = 7.6 Hz, 2H), 4.60 (*t*, J = 7.6 Hz, 2H), 6.72 (*d*, 2Ar–H), 6.91 (*t*, 1Ar–H), 7.21 (*t*, 2Ar–H), 7.66 (*d*, 2Ar–H), 8.48 (*d*, 2Ar–H); ^{13}C NMR (D$_2$O, 100 MHz,): δ = 21.2 (CH$_3$), 29.4 (CH$_2$), 58.5 (CH$_2$), 64.5 (CH$_2$), 114.4 (CH), 121.5 (CH), 128.5 (CH), 129.8 (CH), 143.2 (CH), 157.4 (C), 160.1 (C); IR (KBr) ν_{max} 3132 (C—H Ar), 1600–1470 (C═C), 1167 (C—N), 1078 (C—O) cm^{-1}; LCMS (M^+)–Br$^-$ 228.1 found for C$_{15}$H$_{18}$NO$^+$. Elemental analysis for C$_{15}$H$_{18}$BrNO (308.21); calculated C 58.45, H 5.89, N 4.54%. Found: C 58.51, H 5.82, N 4.49%.

Figure 5
Synthesis of the title compound.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The H atoms were included in idealized positions and treated as riding atoms: C—H = 0.93–0.97 Å with $U_{iso}(H) = 1.5U_{eq}$(C-methyl) and = $1.2U_{eq}$(C) for other H atoms.

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Synthesis and crystal structure of a new pyridinium bromide salt: 4-methyl-1-(3-phenoxypropyl)pyridinium bromide

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO* (Agilent, 2014); data reduction: *CrysAlis PRO* (Agilent, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015) and *WinGX* (Farrugia, 2012).

4-Methyl-1-(3-phenoxypropyl)pyridinium bromide

Crystal data

$C_{15}H_{18}NO^+ \cdot Br^-$	$D_x = 1.407$ Mg m^{-3}
$M_r = 308.21$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Pbca*	Cell parameters from 5457 reflections
$a = 10.3615$ (3) Å	$\theta = 3.2–25.6°$
$b = 13.8916$ (6) Å	$\mu = 2.82$ mm^{-1}
$c = 20.2121$ (8) Å	$T = 295$ K
$V = 2909.29$ (19) Å^3	Prism, colourless
$Z = 8$	$0.60 \times 0.19 \times 0.10$ mm
$F(000) = 1264$	

Data collection

Oxford Diffraction Xcalibur 3/Sapphire3 CCD diffractometer	38980 measured reflections
	2560 independent reflections
Radiation source: Enhance (Mo) X-ray Source	2212 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.048$
Detector resolution: 16.0050 pixels mm^{-1}	$\theta_{max} = 25.0°$, $\theta_{min} = 3.6°$
Thin slice φ and ω scans	$h = -12 \rightarrow 12$
Absorption correction: multi-scan (CrysAlis Pro; Agilent, 2014)	$k = -16 \rightarrow 16$
	$l = -24 \rightarrow 24$
$T_{min} = 0.529$, $T_{max} = 1.000$	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.045$	Secondary atom site location: difference Fourier map
$wR(F^2) = 0.087$	
$S = 1.20$	Hydrogen site location: inferred from neighbouring sites
2560 reflections	
164 parameters	H-atom parameters constrained
0 restraints	

$w = 1/[\sigma^2(F_o^2) + (0.0313P)^2 + 1.5286P]$
    where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.33702 (3)	0.68529 (3)	0.38455 (2)	0.05802 (14)
C1	0.3412 (3)	0.6101 (2)	0.61560 (14)	0.0449 (7)
C2	0.2231 (3)	0.6169 (2)	0.58402 (17)	0.0497 (8)
H2	0.2174	0.6070	0.5386	0.060*
C3	0.1146 (4)	0.6382 (3)	0.6199 (2)	0.0665 (10)
H3	0.0352	0.6421	0.5986	0.080*
C4	0.1213 (4)	0.6540 (3)	0.6864 (2)	0.0768 (12)
H4	0.0471	0.6694	0.7101	0.092*
C5	0.2377 (4)	0.6470 (3)	0.71827 (19)	0.0756 (11)
H5	0.2422	0.6578	0.7636	0.091*
C6	0.3494 (3)	0.6241 (3)	0.68326 (16)	0.0567 (9)
H6	0.4281	0.6182	0.7050	0.068*
O7	0.44380 (18)	0.58949 (16)	0.57589 (10)	0.0516 (6)
C8	0.5707 (3)	0.5894 (2)	0.60379 (14)	0.0487 (8)
H8A	0.5792	0.5381	0.6360	0.058*
H8B	0.5880	0.6503	0.6256	0.058*
C9	0.6631 (3)	0.5744 (2)	0.54734 (16)	0.0514 (8)
H9A	0.6427	0.5145	0.5250	0.062*
H9B	0.7504	0.5696	0.5644	0.062*
C10	0.6554 (3)	0.6566 (2)	0.49855 (15)	0.0478 (7)
H10A	0.5687	0.6602	0.4806	0.057*
H10B	0.6732	0.7167	0.5213	0.057*
N11	0.7491 (2)	0.64405 (17)	0.44343 (11)	0.0400 (6)
C12	0.7086 (3)	0.6251 (2)	0.38199 (15)	0.0440 (7)
H12	0.6206	0.6203	0.3734	0.053*
C13	0.7952 (3)	0.6126 (2)	0.33169 (15)	0.0469 (7)
H13	0.7657	0.5996	0.2892	0.056*
C14	0.9257 (3)	0.6192 (2)	0.34333 (15)	0.0439 (7)
C15	0.9652 (3)	0.6400 (2)	0.40727 (15)	0.0500 (8)
H15	1.0527	0.6449	0.4169	0.060*
C16	0.8761 (3)	0.6533 (2)	0.45620 (16)	0.0493 (8)
H16	0.9033	0.6688	0.4987	0.059*
C17	1.0219 (3)	0.6050 (3)	0.28885 (17)	0.0680 (10)
H17A	1.0431	0.5379	0.2854	0.102*
H17B	1.0986	0.6411	0.2984	0.102*
H17C	0.9856	0.6268	0.2478	0.102*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0428 (2)	0.0664 (2)	0.0649 (2)	−0.00036 (16)	0.00019 (15)	−0.00230 (18)
C1	0.0509 (17)	0.0394 (16)	0.0444 (17)	−0.0034 (14)	0.0090 (15)	0.0015 (14)
C2	0.0513 (18)	0.0434 (19)	0.0544 (18)	0.0051 (15)	0.0028 (16)	0.0044 (15)
C3	0.0530 (19)	0.057 (2)	0.089 (3)	0.0066 (18)	0.014 (2)	0.012 (2)
C4	0.073 (3)	0.068 (3)	0.089 (3)	0.002 (2)	0.043 (2)	0.005 (2)
C5	0.104 (3)	0.069 (3)	0.053 (2)	−0.011 (2)	0.030 (2)	−0.0030 (19)
C6	0.066 (2)	0.062 (2)	0.0421 (18)	−0.0088 (17)	0.0079 (16)	−0.0033 (16)
O7	0.0421 (11)	0.0718 (16)	0.0410 (11)	0.0003 (10)	0.0042 (10)	−0.0120 (11)
C8	0.0472 (17)	0.054 (2)	0.0446 (17)	−0.0009 (15)	−0.0007 (14)	0.0019 (15)
C9	0.0454 (17)	0.0531 (19)	0.0557 (19)	0.0045 (15)	0.0050 (15)	0.0003 (16)
C10	0.0431 (16)	0.0490 (18)	0.0513 (18)	0.0030 (14)	0.0041 (14)	−0.0031 (15)
N11	0.0347 (12)	0.0386 (14)	0.0468 (14)	0.0002 (10)	0.0003 (11)	−0.0012 (11)
C12	0.0374 (15)	0.0456 (18)	0.0489 (18)	−0.0023 (13)	−0.0103 (14)	0.0005 (15)
C13	0.0490 (17)	0.0508 (19)	0.0407 (16)	−0.0033 (15)	−0.0055 (14)	−0.0008 (14)
C14	0.0466 (16)	0.0400 (17)	0.0452 (17)	−0.0042 (14)	0.0036 (14)	0.0014 (14)
C15	0.0324 (15)	0.062 (2)	0.0554 (19)	−0.0070 (15)	−0.0019 (14)	−0.0028 (16)
C16	0.0410 (16)	0.061 (2)	0.0462 (18)	−0.0061 (15)	−0.0059 (14)	−0.0058 (16)
C17	0.062 (2)	0.082 (3)	0.059 (2)	−0.007 (2)	0.0151 (18)	−0.0050 (19)

Geometric parameters (Å, º)

C1—O7	1.362 (3)	C9—H9B	0.9700
C1—C2	1.383 (4)	C10—N11	1.488 (4)
C1—C6	1.384 (4)	C10—H10A	0.9700
C2—C3	1.371 (5)	C10—H10B	0.9700
C2—H2	0.9300	N11—C12	1.337 (3)
C3—C4	1.364 (5)	N11—C16	1.347 (4)
C3—H3	0.9300	C12—C13	1.368 (4)
C4—C5	1.371 (6)	C12—H12	0.9300
C4—H4	0.9300	C13—C14	1.375 (4)
C5—C6	1.393 (5)	C13—H13	0.9300
C5—H5	0.9300	C14—C15	1.386 (4)
C6—H6	0.9300	C14—C17	1.498 (4)
O7—C8	1.431 (3)	C15—C16	1.365 (4)
C8—C9	1.505 (4)	C15—H15	0.9300
C8—H8A	0.9700	C16—H16	0.9300
C8—H8B	0.9700	C17—H17A	0.9600
C9—C10	1.511 (4)	C17—H17B	0.9600
C9—H9A	0.9700	C17—H17C	0.9600
O7—C1—C2	115.6 (3)	N11—C10—C9	111.4 (2)
O7—C1—C6	124.3 (3)	N11—C10—H10A	109.3
C2—C1—C6	120.0 (3)	C9—C10—H10A	109.3
C3—C2—C1	119.8 (3)	N11—C10—H10B	109.3
C3—C2—H2	120.1	C9—C10—H10B	109.3

C1—C2—H2	120.1	H10A—C10—H10B	108.0
C4—C3—C2	120.9 (4)	C12—N11—C16	120.2 (2)
C4—C3—H3	119.5	C12—N11—C10	120.9 (2)
C2—C3—H3	119.5	C16—N11—C10	118.9 (2)
C3—C4—C5	119.8 (4)	N11—C12—C13	120.6 (3)
C3—C4—H4	120.1	N11—C12—H12	119.7
C5—C4—H4	120.1	C13—C12—H12	119.7
C4—C5—C6	120.6 (3)	C12—C13—C14	120.7 (3)
C4—C5—H5	119.7	C12—C13—H13	119.7
C6—C5—H5	119.7	C14—C13—H13	119.7
C1—C6—C5	118.9 (3)	C13—C14—C15	117.6 (3)
C1—C6—H6	120.6	C13—C14—C17	121.3 (3)
C5—C6—H6	120.6	C15—C14—C17	121.1 (3)
C1—O7—C8	119.0 (2)	C16—C15—C14	120.3 (3)
O7—C8—C9	106.6 (2)	C16—C15—H15	119.9
O7—C8—H8A	110.4	C14—C15—H15	119.9
C9—C8—H8A	110.4	N11—C16—C15	120.6 (3)
O7—C8—H8B	110.4	N11—C16—H16	119.7
C9—C8—H8B	110.4	C15—C16—H16	119.7
H8A—C8—H8B	108.6	C14—C17—H17A	109.5
C8—C9—C10	110.9 (3)	C14—C17—H17B	109.5
C8—C9—H9A	109.5	H17A—C17—H17B	109.5
C10—C9—H9A	109.5	C14—C17—H17C	109.5
C8—C9—H9B	109.5	H17A—C17—H17C	109.5
C10—C9—H9B	109.5	H17B—C17—H17C	109.5
H9A—C9—H9B	108.1		
O7—C1—C2—C3	−179.4 (3)	C9—C10—N11—C12	111.0 (3)
C6—C1—C2—C3	0.5 (5)	C9—C10—N11—C16	−69.8 (3)
C1—C2—C3—C4	0.7 (5)	C16—N11—C12—C13	1.5 (4)
C2—C3—C4—C5	−1.0 (6)	C10—N11—C12—C13	−179.3 (3)
C3—C4—C5—C6	0.0 (6)	N11—C12—C13—C14	0.1 (5)
O7—C1—C6—C5	178.5 (3)	C12—C13—C14—C15	−0.8 (5)
C2—C1—C6—C5	−1.4 (5)	C12—C13—C14—C17	179.5 (3)
C4—C5—C6—C1	1.2 (5)	C13—C14—C15—C16	0.0 (5)
C2—C1—O7—C8	174.7 (3)	C17—C14—C15—C16	179.6 (3)
C6—C1—O7—C8	−5.3 (4)	C12—N11—C16—C15	−2.4 (5)
C1—O7—C8—C9	−174.5 (3)	C10—N11—C16—C15	178.4 (3)
O7—C8—C9—C10	62.9 (3)	C14—C15—C16—N11	1.6 (5)
C8—C9—C10—N11	178.4 (2)		

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C10—H10A⋯O7	0.97	2.52	2.850 (3)	100
C10—H10B⋯Br1[i]	0.97	2.89	3.735 (3)	146
C10—H10A⋯Br1	0.97	3.11	4.043 (3)	163
C12—H12⋯Br1	0.93	3.08	3.940 (3)	154

C15—H15···Br1[ii]	0.93	3.07	3.931 (3)	155
C17—H17*B*···Br1[ii]	0.96	3.08	3.956 (4)	152

Symmetry codes: (i) $x+1/2$, $-y+3/2$, $-z+1$; (ii) $x+1$, y, z.