Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Methoxyanilinium bromide

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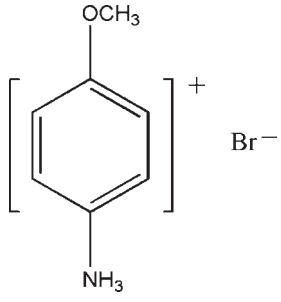
Received 5 August 2009; accepted 31 August 2009

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.043; wR factor = 0.100; data-to-parameter ratio = 21.3.

The title compound, $C_7H_{10}NO^+\cdot Br^-$, consists of almost planar 4-methoxyanilinium cations, wherein the O atom lies 0.049 (3) Å out of the plane formed by the non-H atoms, and a Br^- anion. Strong N—H···Br and N—H···(Br,Br) hydrogen bonding contributes to the stability of the crystal structure and links the cations and anions into a three-dimensional network.

Related literature

For background to dielectric–ferroelectric materials, see: Hang *et al.* (2009); Li *et al.* (2008). For related structures, see: Tan *et al.* (2006); Soumhi *et al.* (2006); Ben Amor *et al.* (1995).



Experimental

Crystal data

$C_7H_{10}NO^+\cdot Br^-$
M_r = 204.07
Orthorhombic, *Pbca*
a = 8.9779 (18) Å
b = 8.6978 (17) Å
c = 22.132 (4) Å
V = 1728.2 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.69 mm^{-1}
T = 298 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.391, T_{max} = 0.391
16334 measured reflections
1985 independent reflections
1276 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.100
S = 1.12
1985 reflections
93 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Br1	0.89	2.52	3.409 (3)	177
N1—H1B···Br1^{i}	0.89	2.55	3.314 (3)	145
N1—H1B···Br1^{ii}	0.89	3.00	3.430 (3)	112
N1—H1C···Br1^{iii}	0.89	2.57	3.300 (3)	140

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *PRPKAPPA* (Ferguson, 1999).

The author is grateful to the starter fund of Southeast University for financial support to buy the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2194).

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supplementary materials

Acta Cryst. (2009). E**65**, o2344 [**doi:10.1107/S160053680903503X**]

4-Methoxyanilinium bromide

X. Fu

Comment

This study is a part of systematic investigation of dielectric-ferroelectric materials, including organic ligands (Li *et al.*, 2008), metal-organic coordination compounds (Hang *et al.*, 2009) and organic-inorganic hybrids. The title compound, 4-methoxyanilinium bromide, (I), has no dielectric disuniform from 80 K to 450 K, (m.p. 458–459 K). In this article, the crystal structure of (I) has been presented.

The asymmetric unit of the title compound is built up from an almost planar 4-methoxybenzenamine cation wherein O1 lies 0.049 (3) Å out of the plane formed by its non-hydrogen atoms and a Br^- anion (Fig. 1). The strong N—H···Br hydrogen bonding (N···Br distances 3.300 (3)–3.430 (3) Å) contribute to the stability of the crystal structure and lead the cations and anions to tridimensional network (Fig 2). The crystal structures containing 4-methoxybenzenamine cation have been reported (Tan *et al.*, 2006; Soumhi *et al.*, 2006; Ben Amor *et al.*, 1995).

Experimental

Single crystals of 4-methoxyanilinium bromide were prepared by slow evaporation at room temperature of an ethanol solution of 4-methoxybenzenamine and hydrobromic acid.

Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

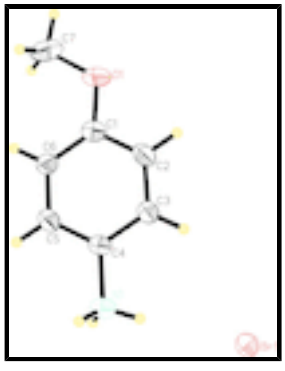

Fig. 1. The molecular structure of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at 30% probability level.

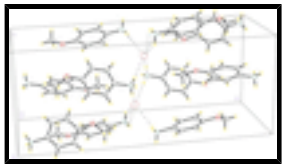

Fig. 2. A view of the packing of the title compound; dashed lines indicate hydrogen bonds.

4-Methoxyanilinium bromide

Crystal data

$C_7H_{10}NO^+·Br^-$	F_{000} = 816
M_r = 204.07	D_x = 1.569 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 6139 reflections
a = 8.9779 (18) Å	θ = 3.3–27.7º
b = 8.6978 (17) Å	μ = 4.69 mm^{-1}
c = 22.132 (4) Å	*T* = 298 K
V = 1728.2 (6) Å^3	Prism, colourless
Z = 8	0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer	1985 independent reflections
Radiation source: fine-focus sealed tube	1276 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.075
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 27.5º
T = 298 K	θ_{min} = 3.4º
ω scans	*h* = −11→11
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	*k* = −11→11
T_{min} = 0.391, T_{max} = 0.391	*l* = −28→28
16334 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.043	$w = 1/[\sigma^2(F_o^2) + (0.0263P)^2 + 1.3429P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.100	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.12	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
1985 reflections	$\Delta\rho_{min}$ = −0.33 e Å^{-3}
93 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Extinction coefficient: 0.0232 (9)

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 $F^2 > \sigma(F^2)$ 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}
O1	0.1517 (3)	0.3060 (4)	0.29591 (13)	0.0721 (9)
N1	0.0282 (4)	0.2527 (4)	0.05037 (14)	0.0548 (9)
H1A	0.0842	0.3201	0.0305	0.066*
H1B	−0.0676	0.2748	0.0447	0.066*
H1C	0.0469	0.1583	0.0369	0.066*
C1	0.1170 (5)	0.2823 (5)	0.23712 (18)	0.0497 (10)
C2	0.1934 (5)	0.3727 (5)	0.1965 (2)	0.0650 (12)
H2A	0.2650	0.4412	0.2105	0.078*
C3	0.1653 (5)	0.3630 (5)	0.13576 (18)	0.0596 (11)
H3A	0.2166	0.4258	0.1088	0.071*
C4	0.0621 (4)	0.2612 (4)	0.11502 (17)	0.0427 (9)
C5	−0.0123 (4)	0.1673 (5)	0.15443 (17)	0.0538 (10)
H5A	−0.0808	0.0958	0.1401	0.065*
C6	0.0153 (5)	0.1797 (5)	0.21591 (17)	0.0533 (11)
H6A	−0.0363	0.1173	0.2429	0.064*
C7	0.0851 (7)	0.2069 (6)	0.3394 (2)	0.0914 (17)
H7A	0.1184	0.2351	0.3791	0.137*
H7B	0.1134	0.1025	0.3312	0.137*
H7C	−0.0213	0.2162	0.3373	0.137*
Br1	0.25218 (4)	0.51025 (4)	−0.021898 (16)	0.0495 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.084 (2)	0.088 (2)	0.0449 (17)	0.0026 (19)	−0.0164 (17)	−0.0048 (17)
N1	0.057 (2)	0.059 (2)	0.0480 (19)	0.0099 (16)	−0.0074 (17)	−0.0047 (15)
C1	0.048 (2)	0.053 (2)	0.048 (2)	0.011 (2)	−0.0035 (19)	−0.006 (2)
C2	0.067 (3)	0.068 (3)	0.060 (3)	−0.021 (2)	−0.008 (2)	−0.009 (2)
C3	0.063 (3)	0.066 (3)	0.050 (3)	−0.017 (2)	−0.001 (2)	−0.001 (2)
C4	0.042 (2)	0.045 (2)	0.041 (2)	0.0082 (17)	−0.0029 (17)	−0.0057 (17)

C5	0.049 (2)	0.054 (3)	0.058 (3)	−0.005 (2)	−0.007 (2)	−0.006 (2)
C6	0.051 (3)	0.061 (3)	0.048 (2)	−0.004 (2)	0.001 (2)	0.0055 (19)
C7	0.107 (4)	0.120 (5)	0.047 (3)	0.011 (4)	−0.007 (3)	0.012 (3)
Br1	0.0493 (3)	0.0461 (3)	0.0531 (3)	0.00163 (19)	−0.0010 (2)	−0.00423 (18)

Geometric parameters (Å, °)

O1—C1	1.354 (5)	C3—C4	1.361 (5)
O1—C7	1.424 (6)	C3—H3A	0.9300
N1—C4	1.465 (5)	C4—C5	1.369 (5)
N1—H1A	0.8893	C5—C6	1.387 (5)
N1—H1B	0.8903	C5—H5A	0.9300
N1—H1C	0.8899	C6—H6A	0.9300
C1—C6	1.360 (6)	C7—H7A	0.9600
C1—C2	1.377 (6)	C7—H7B	0.9600
C2—C3	1.370 (5)	C7—H7C	0.9600
C2—H2A	0.9300		
C1—O1—C7	117.5 (4)	C3—C4—C5	120.4 (4)
C4—N1—H1A	109.5	C3—C4—N1	120.3 (4)
C4—N1—H1B	109.2	C5—C4—N1	119.4 (3)
H1A—N1—H1B	109.5	C4—C5—C6	119.4 (4)
C4—N1—H1C	109.6	C4—C5—H5A	120.3
H1A—N1—H1C	109.6	C6—C5—H5A	120.3
H1B—N1—H1C	109.5	C1—C6—C5	120.6 (4)
O1—C1—C6	125.9 (4)	C1—C6—H6A	119.7
O1—C1—C2	115.2 (4)	C5—C6—H6A	119.7
C6—C1—C2	118.9 (4)	O1—C7—H7A	109.5
C3—C2—C1	120.9 (4)	O1—C7—H7B	109.5
C3—C2—H2A	119.5	H7A—C7—H7B	109.5
C1—C2—H2A	119.5	O1—C7—H7C	109.5
C4—C3—C2	119.7 (4)	H7A—C7—H7C	109.5
C4—C3—H3A	120.1	H7B—C7—H7C	109.5
C2—C3—H3A	120.1		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···Br1	0.89	2.52	3.409 (3)	177
N1—H1B···Br1^{i}	0.89	2.55	3.314 (3)	145
N1—H1B···Br1^{ii}	0.89	3.00	3.430 (3)	112
N1—H1C···Br1^{iii}	0.89	2.57	3.300 (3)	140

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

Fig. 1

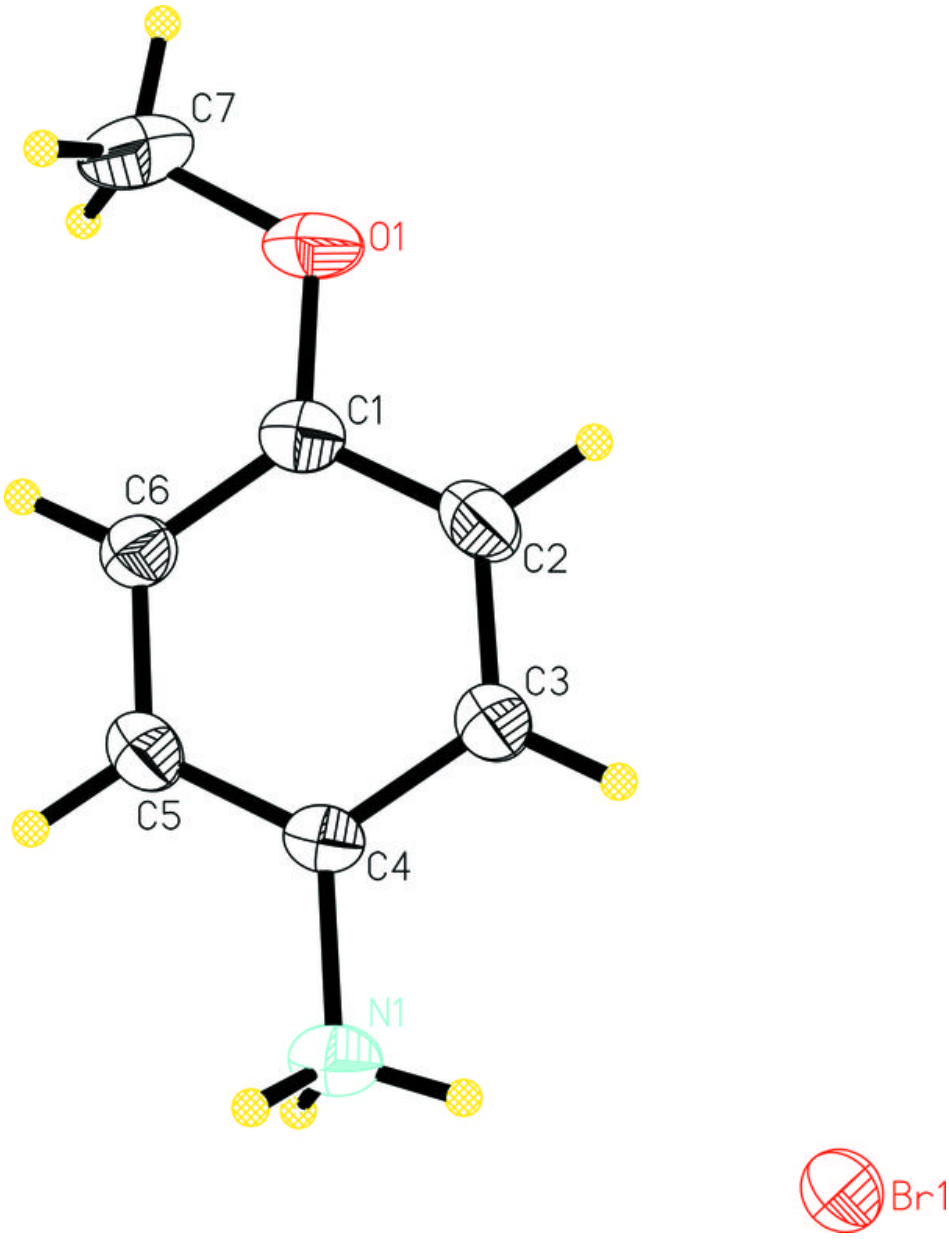

Fig. 2