Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Chloroanilinium bromide

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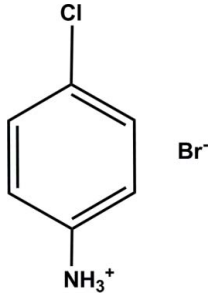
Received 29 May 2012; accepted 1 June 2012

Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.007 Å; R factor = 0.041; wR factor = 0.103; data-to-parameter ratio = 19.8.

In the title compound, $C_6H_7ClN^+\cdot Br^-$, the amino N atom is protonated. All non-H atoms of the cation are essentially coplanar [r.m.s. deviation = 0.004 (3) Å]. In the crystal, N—H···Br hydrogen bonds connect the ions, forming a ribbon-like structure propagating along [010].

Related literature

For the structures and properties of related compounds, see: Fu *et al.* (2011*a*,*b*,*c*); Wang *et al.* (2002); Xue *et al.* (2002); Ye *et al.* (2008).



Experimental

Crystal data

$C_6H_7ClN^+\cdot Br^-$
M_r = 208.49
Triclinic, $P\overline{1}$
a = 4.3989 (2) Å
b = 6.2553 (2) Å
c = 13.8907 (8) Å
α = 91.4000 (8)°
β = 93.580 (1)°
γ = 101.967 (1)°
V = 372.91 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 5.78 mm^{-1}
T = 153 K
0.10 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.910, T_{max} = 1.000
3843 measured reflections
1647 independent reflections
1435 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.103
S = 1.11
1647 reflections
83 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −1.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Br1^{i}	0.89	2.59	3.467 (4)	167
N1—H1B···Br1^{ii}	0.89	2.52	3.370 (4)	161
N1—H1C···Br1^{iii}	0.89	2.46	3.312 (4)	161

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

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: *SHELXTL*.

This work was supported by a start–up grant from Southeast University, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AA2066).

References

Fu, D.-W., Zhang, W., Cai, H.-L., Zhang, Y., Ge, J.-Z., Xiong, R.-G. & Huang, S. P. D. (2011*a*). *J. Am. Chem. Soc.* **133**, 12780–12786.
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supplementary materials

Acta Cryst. (2012). E**68**, o2022 [doi:10.1107/S1600536812024993]

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Comment

Simple organic salts containing strong intrermolecular H–bonds have attracted an attention as materials which display ferroelectric–paraelectric phase transitions (Fu *et al.*, 2011*a*, *b*, *c*). With the purpose of obtaining phase transition crystals of organic salts, various organic molecules have been studied and a series of new crystal materials have been elaborated (Wang *et al.*, 2002; Xue *et al.*, 2002; Ye *et al.*, 2008).

In the title compound (Fig. 1), the bond lengths and angles have normal values. The asymmetric unit is composed of one 4-chloroanilinium cation and one Br^- anion. The protonated N atom is involved in strong intermolecular N—H···Br hydrogen bonds (Table 1) which connect the ions into a 2D network parallel to the *ab*–plane (Fig. 2). The crystal packing is further stabilized by aromatic π–π interactions between the benzene rings of the neighbouring cations with the Cg···Cg distances of 4.399 (1)Å (Cg is the centroid of the benzene ring).

Experimental

The HBr (1 mL, 2 mol/L), 4-chloroaniline (10 mmol) and ethanol (50 mL) were added into a 100 mL flask. The mixture was stirred at 333 K for 2 h, and then the precipitate was filtered out. Colourless crystals suitable for X–ray diffraction were obtained by slow evaporation of the solution.

Refinement

All the H atoms attached to C atoms were placed into the idealized positions and treated as riding with C—H = 0.93Å (aromatic) and U_{iso}(H) = 1.2U_{eq}(C). The H atoms based on N were placed into the calculated positions with the N—H = 0.89Å and refined with U_{iso}(H) = 1.5U_{eq}(N).

Computing details

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

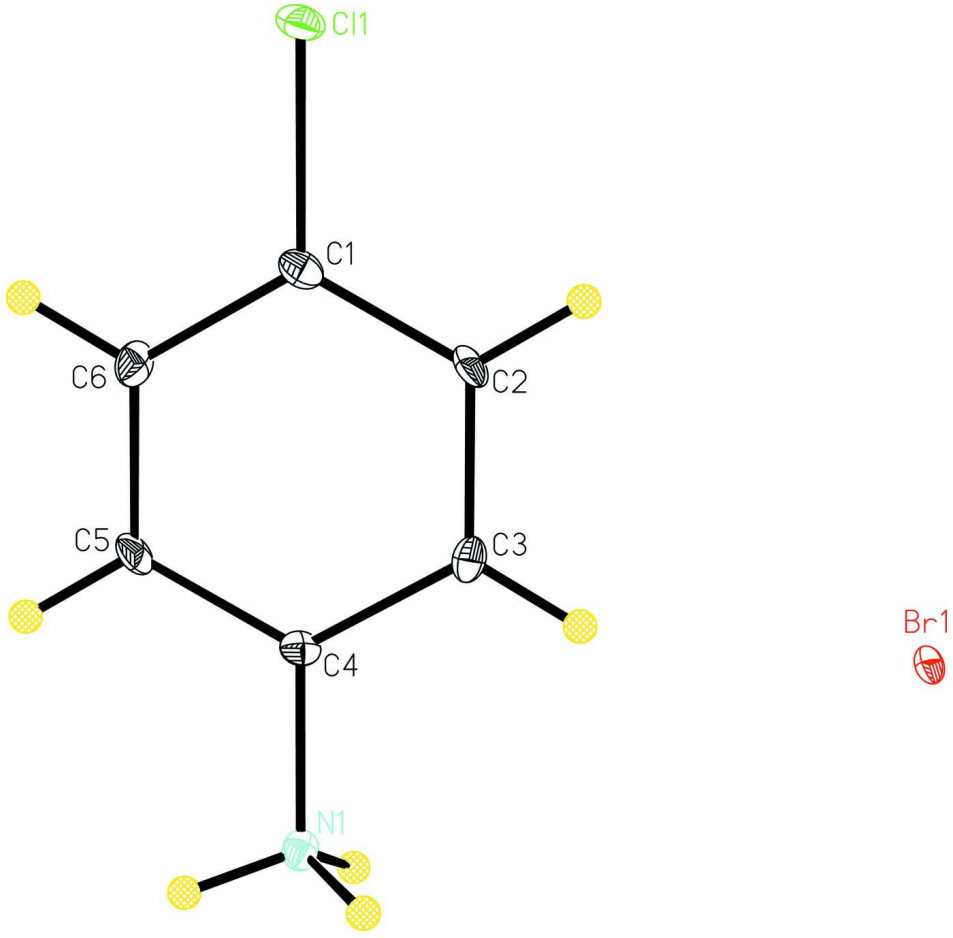

Figure 1

A view of the asymmetric unit with the atomic numbering scheme. The displacement ellipsoids were drawn at the 30% probability level.

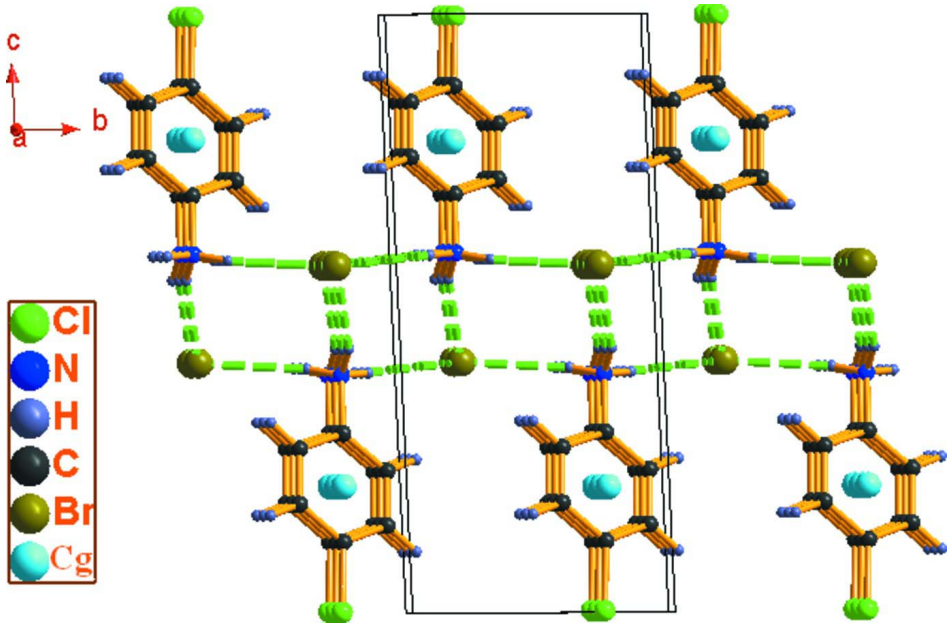

Figure 2

The crystal packing of the title compound viewed along the *a* axis showing the H–bonding and π–π interactions (dashed line), Cg is the centroid of the benzene ring.

4-Chloroanilinium bromide

Crystal data

$C_6H_7ClN^+\cdot Br^-$
$M_r = 208.49$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 4.3989$ (2) Å
$b = 6.2553$ (2) Å
$c = 13.8907$ (8) Å
$\alpha = 91.4000$ (8)°
$\beta = 93.580$ (1)°
$\gamma = 101.967$ (1)°
$V = 372.91$ (3) Å^3
$Z = 2$
$F(000) = 204$
$D_x = 1.857$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1674 reflections
$\theta = 3.0$–27.5°
$\mu = 5.78$ mm^{-1}
$T = 153$ K
Block, colourless
0.10 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD profile fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.910$, $T_{max} = 1.000$
3843 measured reflections
1647 independent reflections
1435 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 27.5$°, $\theta_{min} = 2.9$°
$h = -5\rightarrow5$
$k = -8\rightarrow8$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.103$
$S = 1.11$
1647 reflections
83 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
$w = 1/[\sigma^2(F_o^2) + (0.044P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.84$ e Å^{-3}
$\Delta\rho_{min} = -1.47$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s 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 $F^2 > 2$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}
Cl1	0.6759 (3)	0.27570 (19)	0.99710 (9)	0.0205 (3)
N1	1.1049 (9)	0.2261 (6)	0.6017 (3)	0.0136 (8)
H1A	1.2142	0.1217	0.5980	0.020*
H1B	1.2258	0.3545	0.5904	0.020*
H1C	0.9437	0.1973	0.5580	0.020*
C1	0.7915 (11)	0.2566 (8)	0.8806 (4)	0.0154 (10)
Br1	0.41356 (10)	0.76145 (7)	0.58041 (3)	0.01335 (18)
C2	0.7543 (11)	0.4182 (7)	0.8164 (3)	0.0155 (10)
H2A	0.6637	0.5329	0.8352	0.019*
C3	0.8537 (11)	0.4061 (7)	0.7241 (4)	0.0151 (10)
H3A	0.8289	0.5113	0.6798	0.018*
C4	0.9907 (10)	0.2340 (7)	0.6991 (3)	0.0113 (9)
C5	1.0258 (11)	0.0722 (7)	0.7620 (3)	0.0151 (10)
H5A	1.1156	−0.0428	0.7430	0.018*
C6	0.9254 (11)	0.0842 (7)	0.8533 (4)	0.0159 (10)
H6A	0.9471	−0.0233	0.8968	0.019*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0316 (7)	0.0169 (6)	0.0146 (6)	0.0075 (5)	0.0080 (5)	−0.0018 (5)
N1	0.018 (2)	0.011 (2)	0.012 (2)	0.0037 (16)	−0.0009 (17)	−0.0014 (16)
C1	0.017 (2)	0.014 (2)	0.015 (3)	0.0028 (19)	0.002 (2)	−0.0045 (19)
Br1	0.0165 (3)	0.0087 (3)	0.0154 (3)	0.00395 (18)	0.00213 (18)	−0.00161 (17)
C2	0.020 (2)	0.011 (2)	0.018 (3)	0.0072 (19)	0.004 (2)	−0.0033 (19)
C3	0.018 (2)	0.009 (2)	0.019 (3)	0.0018 (19)	0.001 (2)	0.0029 (19)

C4	0.013 (2)	0.009 (2)	0.010 (2)	−0.0007 (17)	0.0002 (18)	−0.0041 (18)
C5	0.019 (2)	0.011 (2)	0.017 (3)	0.0065 (19)	0.003 (2)	−0.0043 (19)
C6	0.023 (3)	0.008 (2)	0.016 (3)	0.0023 (19)	−0.001 (2)	0.0000 (19)

Geometric parameters (Å, º)

Cl1—C1	1.735 (5)	C2—H2A	0.9300
N1—C4	1.476 (6)	C3—C4	1.385 (6)
N1—H1A	0.8900	C3—H3A	0.9300
N1—H1B	0.8900	C4—C5	1.379 (6)
N1—H1C	0.8900	C5—C6	1.375 (7)
C1—C6	1.388 (6)	C5—H5A	0.9300
C1—C2	1.392 (6)	C6—H6A	0.9300
C2—C3	1.385 (7)		
C4—N1—H1A	109.5	C4—C3—C2	118.6 (4)
C4—N1—H1B	109.5	C4—C3—H3A	120.7
H1A—N1—H1B	109.5	C2—C3—H3A	120.7
C4—N1—H1C	109.5	C5—C4—C3	122.5 (4)
H1A—N1—H1C	109.5	C5—C4—N1	119.2 (4)
H1B—N1—H1C	109.5	C3—C4—N1	118.3 (4)
C6—C1—C2	120.9 (5)	C6—C5—C4	118.7 (4)
C6—C1—Cl1	119.8 (4)	C6—C5—H5A	120.6
C2—C1—Cl1	119.2 (4)	C4—C5—H5A	120.6
C3—C2—C1	119.3 (4)	C5—C6—C1	120.0 (4)
C3—C2—H2A	120.4	C5—C6—H6A	120.0
C1—C2—H2A	120.4	C1—C6—H6A	120.0

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Br1^{i}	0.89	2.59	3.467 (4)	167
N1—H1*B*···Br1^{ii}	0.89	2.52	3.370 (4)	161
N1—H1*C*···Br1^{iii}	0.89	2.46	3.312 (4)	161

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