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2-Amino-5-bromopyridinium 2-phenoxyacetate

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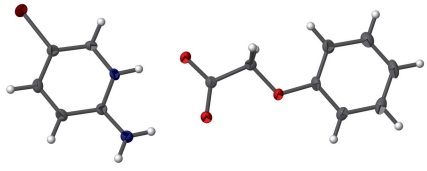
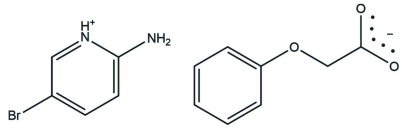
The phenoxyacetate anion of the title salt, $C_5H_6BrN_2^+\cdot C_8H_7O_3^-$, is essentially planar, with a dihedral angle of 7.6 (5)° between the carboxylate group and the benzene ring. In the crystal, the cation and the anion are linked *via* N—H···O hydrogen bonds, forming a helical chain along a 2_1 screw axis. In the chain, a π–π stacking interaction between the pyridinium and benzene rings, with a centroid–centroid distance of 3.854 (2) Å, and a C—H···O interaction are observed. The chains are further linked through another C—H···O hydrogen bond, forming a three-dimensional network.

3D view



Chemical scheme



Structure description

Supramolecular architectures assembled *via* various delicate non-covalent interactions, such as hydrogen bonds, π–π stacking and electrostatic interactions, *etc*. have attracted intense interest in recent years because of their fascinating structural diversity and potential applications for functional materials (Desiraju, 2007). In particular, the application of intermolecular hydrogen bonds is a well known and efficient tool in the field of organic crystal design owing to its strength and directional properties (Aakeröy & Seddon, 1993). Pyridine and its derivatives play an important role in heterocyclic chemistry (Pozharski *et al.*, 1997; Katritzky *et al.*, 1996). They are often involved in hydrogen-bond interactions. Aryloxyacetic acid derivatives possess a wide array of diverse bioactivities including antimycobacterial (Ali & Shanharyar, 2007; Shaharyar *et al.*, 2006), anti-inflammatory and antioxidant (Kunsch *et al.*, 2005), antibacterial (Iqbal *et al.*, 2007), antilipaemic and antiplatelet (Pérez-Pastén *et al.*, 2006) and inhibitory activity of cathepsin K and aldose reductase (Shinozuka *et al.*, 2006). In order to study some hydrogen-bonding interactions, the structure of the title salt was determined.

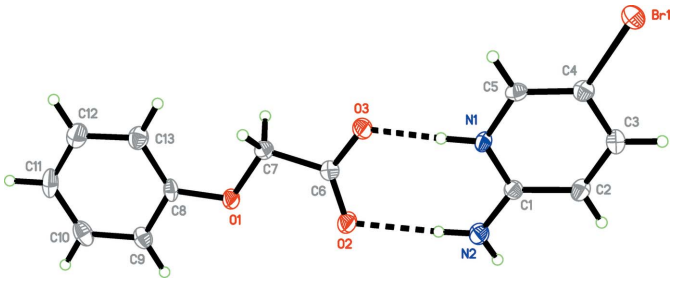


Figure 1
The molecular structure of the title compound, showing the atom labels and 50% probability displacement ellipsoids. Hydrogen bonds are shown as dashed lines.

The asymmetric unit (Fig. 1) contains one 2-amino-5-bromopyridinium cation and one phenoxyacetate anion, in which the carboxyl group of the phenoxyacetate acid is ionized by proton transfer to the nitrogen atom of bromopyridine. The carboxylate anion is also confirmed by the bond distances O2—C6 = 1.242 (4) Å and O3—C6 = 1.270 (4) Å. In the 2-amino-5-bromopyridinium cation, a wider than normal angle [C1—N1—C5 = 122.1 (3)°] is subtended at the protonated N1 atom. This type of protonation is observed in various aminopyridine acid complexes (Hemamalini & Fun 2010; Khalib *et al.*, 2013). The non-H atoms of the 2-amino-5-bromopyridinium cation are essentially co-planar, with a maximum deviation of 0.016 (3) Å for atom N2. The dihedral angle between the pyridine (N1/C1–C5) and benzene (C8–C13) rings is 10.22 (18)°. The anion is essentially planar, with a dihedral angle of 7.6 (5)° between the benzene (C8–C13) ring and the carboxylate (O2/O3/C6) group and with a C8—O1—C7—C6 torsion angle of 172.7 (3)°. All the bond lengths and angles are normal.

In the crystal, the cation and the anion are linked *via* N1—H1*N*1···O3 and N2—H1*N*2···O2 hydrogen bonds, forming an $R_2^2(8)$ ring motif. The cation further interacts with the anions through a bifurcated N2—H2*N*2···(O1^{i},O2^{i}) hydrogen bond and a C2—H2*A*···O2^{i} interaction (symmetry code in Table 1) with $R_1^2(5)$ and $R_2^1(6)$ ring motifs, forming a helical chain (Fig. 2). A π–π stacking interaction between the pyridinium (C1–C5/N1) and benzene (C8–C13; symmetry code: x, $y-1$, z) rings with a centroid–centroid distance of 3.854 (2) Å is observed in the chain. Finally, a weak C5—H5*A*···O3^{ii} hydrogen bond (symmetry code in Table 1), leads to the formation of a three-dimensional network.

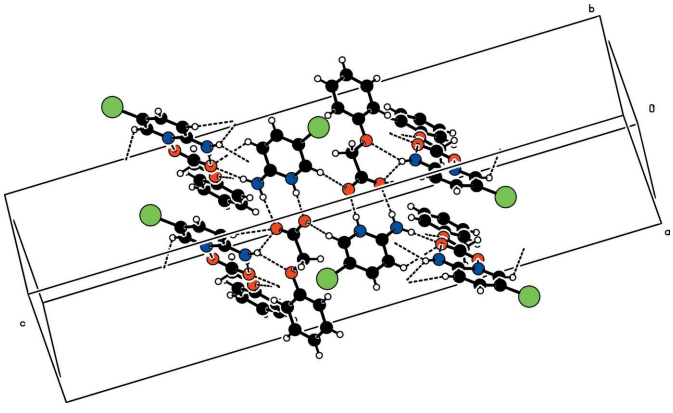


Figure 2
A partial packing diagram of the title compound. The N—H···O and C—H···O hydrogen bonds are shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···O3	0.88 (1)	1.70 (3)	2.579 (4)	176 (5)
N2—H1*N*2···O2	0.87 (1)	2.01 (3)	2.877 (4)	177 (4)
N2—H2*N*2···O1^{i}	0.87 (1)	2.41 (3)	3.140 (4)	142 (5)
N2—H2*N*2···O2^{i}	0.87 (1)	2.13 (3)	2.900 (4)	146 (5)
C2—H2*A*···O2^{i}	0.95	2.55	3.193 (4)	125
C5—H5*A*···O3^{ii}	0.95	2.42	3.047 (4)	123

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{5}{4}$; (ii) $y, x, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_5H_6BrN_2^+\cdot C_8H_7O_3^-$
M_r	325.16
Crystal system, space group	Tetragonal, $P4_12_12$
Temperature (K)	100
a, c (Å)	8.6944 (1), 35.2843 (7)
V (Å^3)	2667.23 (7)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.09
Crystal size (mm)	0.34 × 0.21 × 0.13
Data collection	
Diffractometer	Bruker SMART APEXII CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.419, 0.688
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38666, 3407, 2790
R_{int}	0.076
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.673
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.078, 1.17
No. of reflections	3407
No. of parameters	184
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.52, −0.52
Absolute structure	Flack (1983), 1324 Fridel pairs
Absolute structure parameter	0.072 (13)

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Synthesis and crystallization

A hot methanol solution (20 ml) of 2-amino-5-bromopyridine (43 mg, Aldrich) and phenoxyacetic acid (38 mg, Merck) were mixed and warmed over a heating magnetic-stirrer hotplate for a few minutes. The resulting solution was allowed to cool

slowly at room temperature and crystals of the title compound appeared after a few days.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161939 [https://doi.org/10.1107/S2414314616019398]

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2-Amino-5-bromopyridinium 2-phenoxyacetate

Crystal data

$C_5H_6BrN_2^+·C_8H_7O_3^-$
M_r = 325.16
Tetragonal, $P4_12_12$
Hall symbol: P 4abw 2nw
a = 8.6944 (1) Å
c = 35.2843 (7) Å
V = 2667.23 (7) Å^3
Z = 8
F(000) = 1312
D_x = 1.620 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9890 reflections
θ = 2.3–26.4°
μ = 3.09 mm^{-1}
T = 100 K
Block, colourless
0.34 × 0.21 × 0.13 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.419, T_{max} = 0.688
38666 measured reflections
3407 independent reflections
2790 reflections with $I > 2\sigma(I)$
R_{int} = 0.076
θ_{max} = 28.6°, θ_{min} = 2.3°
h = −11→11
k = −11→11
l = −47→47

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.078
S = 1.17
3407 reflections
184 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 4.511P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Absolute structure: Flack (1983), 1324 Fridel pairs
Absolute structure parameter: 0.072 (13)

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
Br1	0.85535 (5)	1.53676 (5)	0.471862 (11)	0.02404 (10)
O1	1.0287 (3)	0.5443 (3)	0.58802 (7)	0.0207 (6)
O2	0.8557 (3)	0.7960 (3)	0.58999 (7)	0.0251 (6)
O3	0.9831 (3)	0.9012 (3)	0.54112 (7)	0.0228 (6)
N1	0.8335 (3)	1.1573 (4)	0.54085 (8)	0.0168 (6)
N2	0.7130 (4)	1.0932 (4)	0.59699 (10)	0.0218 (7)
C1	0.7426 (4)	1.1976 (4)	0.57033 (10)	0.0171 (8)
C2	0.6803 (4)	1.3478 (5)	0.57085 (10)	0.0204 (8)
H2A	0.6154	1.3790	0.5911	0.024*
C3	0.7137 (4)	1.4481 (5)	0.54222 (11)	0.0220 (8)
H3A	0.6727	1.5494	0.5426	0.026*
C4	0.8083 (4)	1.4014 (4)	0.51234 (10)	0.0193 (8)
C5	0.8671 (4)	1.2562 (4)	0.51232 (10)	0.0177 (7)
H5A	0.9322	1.2241	0.4922	0.021*
C6	0.9580 (5)	0.7964 (4)	0.56542 (10)	0.0177 (8)
C7	1.0704 (4)	0.6625 (4)	0.56195 (10)	0.0196 (8)
H7A	1.0683	0.6216	0.5358	0.024*
H7B	1.1761	0.6986	0.5674	0.024*
C8	1.1075 (4)	0.4079 (4)	0.58550 (10)	0.0178 (8)
C9	1.0630 (5)	0.2962 (4)	0.61188 (10)	0.0211 (9)
H9A	0.9848	0.3175	0.6299	0.025*
C10	1.1351 (5)	0.1534 (5)	0.61129 (11)	0.0254 (9)
H10A	1.1049	0.0769	0.6290	0.030*
C11	1.2500 (5)	0.1206 (5)	0.58536 (11)	0.0277 (10)
H11A	1.2991	0.0230	0.5854	0.033*
C12	1.2921 (5)	0.2316 (5)	0.55947 (12)	0.0283 (10)
H12A	1.3699	0.2092	0.5414	0.034*
C13	1.2226 (5)	0.3765 (5)	0.55927 (11)	0.0235 (9)
H13A	1.2535	0.4524	0.5415	0.028*
H1N1	0.881 (5)	1.068 (3)	0.5407 (12)	0.044 (14)*
H1N2	0.754 (5)	1.002 (3)	0.5955 (13)	0.048 (16)*
H2N2	0.665 (5)	1.123 (6)	0.6174 (9)	0.066 (18)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0268 (2)	0.0230 (2)	0.02226 (17)	0.00121 (18)	0.00088 (18)	0.00592 (17)
O1	0.0260 (14)	0.0159 (13)	0.0203 (13)	0.0051 (13)	0.0058 (12)	0.0047 (11)
O2	0.0299 (16)	0.0215 (14)	0.0241 (13)	0.0079 (13)	0.0103 (13)	0.0050 (11)
O3	0.0276 (16)	0.0194 (14)	0.0215 (13)	0.0050 (12)	0.0059 (12)	0.0068 (11)
N1	0.0152 (16)	0.0165 (16)	0.0185 (14)	0.0039 (13)	−0.0002 (12)	0.0002 (13)
N2	0.0267 (19)	0.0196 (18)	0.0191 (17)	0.0015 (14)	0.0049 (15)	−0.0023 (14)
C1	0.0165 (19)	0.0163 (19)	0.0184 (19)	−0.0002 (15)	−0.0003 (15)	−0.0009 (15)
C2	0.021 (2)	0.022 (2)	0.0188 (17)	0.0049 (16)	0.0010 (15)	−0.0012 (16)
C3	0.024 (2)	0.017 (2)	0.0245 (19)	0.0036 (17)	−0.0018 (16)	0.0000 (16)
C4	0.020 (2)	0.020 (2)	0.0173 (17)	−0.0003 (15)	0.0007 (15)	−0.0013 (15)
C5	0.0171 (19)	0.0211 (19)	0.0149 (16)	−0.0009 (15)	0.0034 (15)	−0.0011 (15)
C6	0.0188 (19)	0.0177 (18)	0.0167 (18)	0.0003 (16)	−0.0011 (16)	−0.0006 (14)
C7	0.023 (2)	0.018 (2)	0.0177 (17)	0.0005 (16)	0.0042 (15)	−0.0003 (15)
C8	0.021 (2)	0.0114 (17)	0.0208 (18)	0.0018 (14)	−0.0052 (16)	−0.0048 (15)
C9	0.028 (2)	0.0173 (19)	0.0186 (18)	−0.0009 (16)	−0.0017 (16)	0.0010 (15)
C10	0.031 (2)	0.0176 (19)	0.028 (2)	−0.001 (2)	−0.0101 (18)	0.0037 (17)
C11	0.029 (2)	0.018 (2)	0.036 (2)	0.0082 (18)	−0.0110 (19)	−0.0085 (18)
C12	0.028 (2)	0.026 (2)	0.032 (2)	0.0052 (19)	0.0004 (19)	−0.0031 (19)
C13	0.026 (2)	0.022 (2)	0.023 (2)	0.0039 (17)	−0.0006 (17)	0.0008 (17)

Geometric parameters (Å, º)

Br1—C4	1.895 (4)	C4—C5	1.362 (5)
O1—C8	1.372 (4)	C5—H5A	0.9500
O1—C7	1.427 (4)	C6—C7	1.524 (5)
O2—C6	1.242 (4)	C7—H7A	0.9900
O3—C6	1.270 (4)	C7—H7B	0.9900
N1—C1	1.353 (5)	C8—C13	1.390 (5)
N1—C5	1.356 (4)	C8—C9	1.400 (5)
N1—H1N1	0.876 (10)	C9—C10	1.390 (5)
N2—C1	1.332 (5)	C9—H9A	0.9500
N2—H1N2	0.872 (10)	C10—C11	1.384 (6)
N2—H2N2	0.870 (10)	C10—H10A	0.9500
C1—C2	1.414 (5)	C11—C12	1.379 (6)
C2—C3	1.366 (5)	C11—H11A	0.9500
C2—H2A	0.9500	C12—C13	1.398 (6)
C3—C4	1.398 (5)	C12—H12A	0.9500
C3—H3A	0.9500	C13—H13A	0.9500
C8—O1—C7	117.0 (3)	O1—C7—C6	109.6 (3)
C1—N1—C5	122.1 (3)	O1—C7—H7A	109.7
C1—N1—H1N1	121 (3)	C6—C7—H7A	109.7
C5—N1—H1N1	117 (3)	O1—C7—H7B	109.7
C1—N2—H1N2	120 (3)	C6—C7—H7B	109.7
C1—N2—H2N2	118 (4)	H7A—C7—H7B	108.2

H1N2—N2—H2N2	121 (5)	O1—C8—C13	124.9 (3)
N2—C1—N1	118.6 (3)	O1—C8—C9	114.8 (3)
N2—C1—C2	123.1 (3)	C13—C8—C9	120.3 (3)
N1—C1—C2	118.2 (3)	C10—C9—C8	119.0 (4)
C3—C2—C1	119.9 (3)	C10—C9—H9A	120.5
C3—C2—H2A	120.0	C8—C9—H9A	120.5
C1—C2—H2A	120.0	C11—C10—C9	121.3 (4)
C2—C3—C4	119.8 (4)	C11—C10—H10A	119.4
C2—C3—H3A	120.1	C9—C10—H10A	119.4
C4—C3—H3A	120.1	C12—C11—C10	119.0 (4)
C5—C4—C3	119.4 (3)	C12—C11—H11A	120.5
C5—C4—Br1	119.6 (3)	C10—C11—H11A	120.5
C3—C4—Br1	121.0 (3)	C11—C12—C13	121.3 (4)
N1—C5—C4	120.5 (3)	C11—C12—H12A	119.3
N1—C5—H5A	119.8	C13—C12—H12A	119.3
C4—C5—H5A	119.8	C8—C13—C12	119.0 (4)
O2—C6—O3	126.6 (4)	C8—C13—H13A	120.5
O2—C6—C7	120.9 (3)	C12—C13—H13A	120.5
O3—C6—C7	112.6 (3)		

C5—N1—C1—N2	179.0 (3)	O3—C6—C7—O1	−175.6 (3)
C5—N1—C1—C2	0.6 (5)	C7—O1—C8—C13	−0.9 (5)
N2—C1—C2—C3	−179.0 (4)	C7—O1—C8—C9	179.6 (3)
N1—C1—C2—C3	−0.5 (5)	O1—C8—C9—C10	179.3 (3)
C1—C2—C3—C4	0.5 (6)	C13—C8—C9—C10	−0.3 (6)
C2—C3—C4—C5	−0.5 (6)	C8—C9—C10—C11	0.4 (6)
C2—C3—C4—Br1	179.3 (3)	C9—C10—C11—C12	−0.7 (6)
C1—N1—C5—C4	−0.5 (5)	C10—C11—C12—C13	0.8 (6)
C3—C4—C5—N1	0.5 (5)	O1—C8—C13—C12	−179.1 (4)
Br1—C4—C5—N1	−179.3 (3)	C9—C8—C13—C12	0.5 (6)
C8—O1—C7—C6	172.7 (3)	C11—C12—C13—C8	−0.7 (6)
O2—C6—C7—O1	4.5 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*1···O3	0.88 (1)	1.70 (3)	2.579 (4)	176 (5)
N2—H1*N*2···O2	0.87 (1)	2.01 (3)	2.877 (4)	177 (4)
N2—H2*N*2···O1^{i}	0.87 (1)	2.41 (3)	3.140 (4)	142 (5)
N2—H2*N*2···O2^{i}	0.87 (1)	2.13 (3)	2.900 (4)	146 (5)
C2—H2*A*···O2^{i}	0.95	2.55	3.193 (4)	125
C5—H5*A*···O3^{ii}	0.95	2.42	3.047 (4)	123

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+5/4; (ii) *y*, *x*, −*z*+1.