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1,3-Bis(4-bromophenyl)-1*H*-imidazol-3-ium tetrafluoroborate

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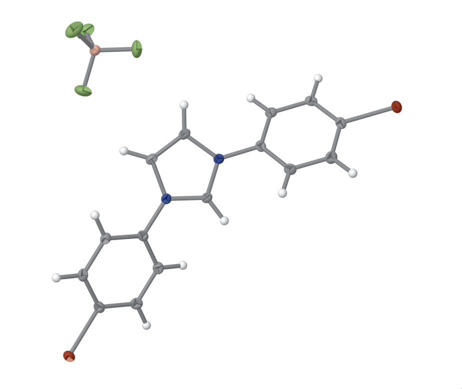
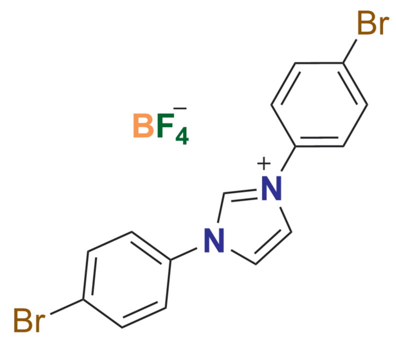
The crystal of the title salt, $C_{15}H_{11}Br_2N_2^+ \cdot BF_4^-$, contains one half of a 1,3-bis(4-bromophenyl)imidazolium cation and one half of a tetrafluoroborate anion in the asymmetric unit; the complete ions are generated by crystallographic twofold symmetry. The imidazolium cation adopts a *syn*-periplanar conformation, with the 4-bromophenyl rings inclined to the central imidazolium ring by 36.04 (4)°. In the crystal, the tetrafluoroborate anion participates in structure-directing halogen-bonding contacts through F⋯Br and F⋯π(phenyl) interactions. These are complemented by intermolecular π–π and Br⋯π interactions, which assemble the ions into two-dimensional supramolecular sheets lying parallel to the *ac* plane. The sheets are further linked by C—H⋯F hydrogen bonds, forming ring motifs of graph sets $R_2^2(7)$ and $R_1^2(4)$ within a three-dimensional supramolecular network.

3D view



Chemical scheme



Structure description

The title compound is a 1,3-diarylsubstituted imidazolium salt, which was originally synthesized *via* a method involving mechano-grinding and acidification (Ikhile *et al.*, 2011). The synthetic method employed herein is a 'green' modification of the initial method (Arduengo *et al.*, 1992). While the synthesis of the title compound has been reported (Ikhile *et al.*, 2011), crystallographic details and those of analogous 1,3-bis(4-halophenyl)imidazolium tetrafluoroborates are not available. The title compound and its related analogues bearing ferrocenyl moieties have found application as green catalysts for the transfer hydrogenation of ketones (Ikhile *et al.*, 2012, 2013). Recent work on similar 1,3-diarylimidazoliumm salts (Ndlovu *et al.*, 2017) and reviews on the biological activity of non-heteroatom functionalized azolium salts (Patil *et al.*, 2020; Fletcher *et al.*, 2018; Mercs & Albrecht, 2010) have also provided evidence on the structure/activity trends in their well established potential as anti-fungal, anti-bacterial and anti-prolif-

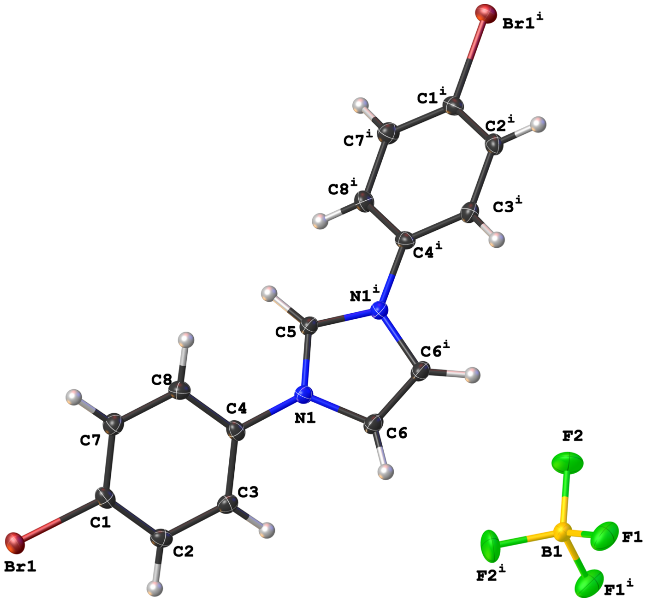


Figure 1
Molecular structure of the title compound showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. Symmetry code: (i) $-x + 1, y, -z + \frac{3}{2}$.

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D\cdots A$	D—H$\cdots$$A$
C5—H5$\cdots$F1^{i}	0.95	2.29	3.156 (2)	151
C6—H6$\cdots$F2^{ii}	0.95	2.39	3.1854 (19)	140

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{11}Br_2N_2^+ \cdot BF_4^-$
M_r	465.89
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	100
a, b, c (Å)	9.5407 (2), 9.8272 (2), 17.0451 (3)
β (°)	102.878 (1)
V (Å^3)	1557.92 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.25
Crystal size (mm)	0.37 × 0.28 × 0.21
Data collection	
Diffractometer	Bruker SMART APEXII area detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.618, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9293, 1922, 1748
R_{int}	0.023
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.017, 0.038, 1.06
No. of reflections	1922
No. of parameters	110
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.29

Computer programs: *APEX2*, *COSMO* and *SAINT* (Bruker, 2009), *SHELXS2013* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

erative agents. As part of our work in developing new imidazolium derivatives with impressive anti-microbial activities (Kadafour *et al.*, 2022; Ndlovu *et al.*, 2017), we synthesized the title compound and determined its crystal structure.

The asymmetric unit of the title compound comprises half a cationic 1,3-bis(4-bromophenyl)imidazolium species and half a tetrafluoroborate counter-ion, with the complete ions being generated by a C_2 rotation axis that runs parallel to the C5—H5 bond (Fig. 1). The cationic species adopts a *syn*-periplanar conformation with the dihedral angle between the mean planes of the central imidazolium ring and the 4-bromophenyl wingtip being 36.04 (4)°, which is wider than that observed in the hydrated chloride analogue of the title compound, *i.e.* 2.9 (1)° (Garden *et al.*, 2010).

The extended structure features halogen bonding that is driven by the tetrafluoroborate moiety *via* F1$\cdots$$\pi$(phenyl) [F1$\cdots$$Cg$(phenyl) = 3.5669 (12) Å, symmetry operation: $\frac{3}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$ and F2$\cdots$Br1 (F2$\cdots$Br1 = 2.8890 (12) Å, symmetry code: $\frac{1}{2} + x, \frac{3}{2} - y, -\frac{1}{2} + z$] interactions. In conjunction with the halogen-bonding patterns involving F atoms, intermolecular π(phenyl)–π(phenyl) [$Cg\cdots Cg$ = 3.6720 (9) Å, symmetry operation: $1 - x, 1 - y, 1 - z$] and π(phenyl)$\cdots$Br1 [Br$\cdots\pi$ = 3.9061 (6) Å, symmetry operation: $1 - x, 1 - y$, 1-*z*; $x, 1 - y, -\frac{1}{2} - z$) interactions occur within two-dimensional supramolecular networks parallel to the *ac* plane (Fig. 2). Finally, intermolecular C—H$\cdots$F hydrogen bonds with graph-set descriptors $R_2^2(7)$ and $R_1^2(4)$, link the two-dimensional supramolecular networks along the *b* axis within a three-dimensional framework (Table 1, Fig. 3).

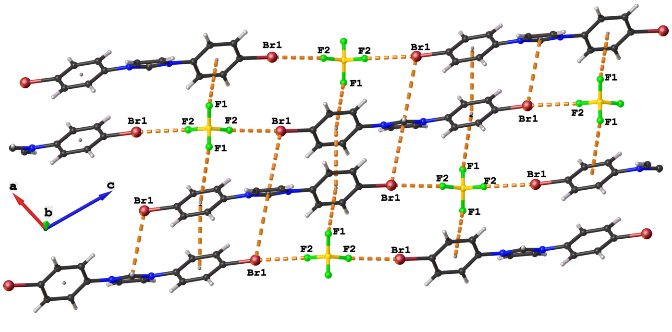


Figure 2
Representation of π(phenyl)–π(phenyl), π(phenyl)$\cdots$Br and F$\cdots$Br interactions in the crystal of the title compound.

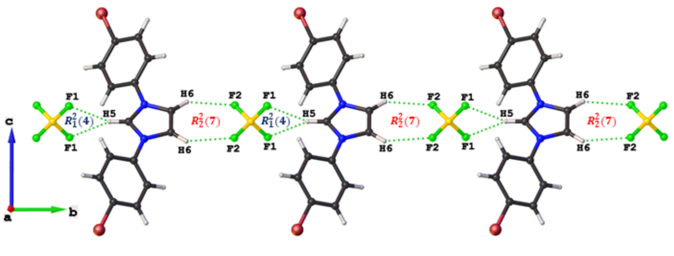


Figure 3
Representation of C—H$\cdots$F hydrogen bonds in the crystal of the title compound.

Synthesis and crystallization

The details on the synthesis of the title compound have been reported (Ikhile *et al.*, 2011). The starting materials were 1,3-bis(4-bromophenyl)ethylenediimine (1.5 g; 4.10 mmol), paraformaldehyde (0.123 g: 4.10 mmol) and HBF_4 (0.54 ml; 0.36 g; 4.10 mmol). Brown precipitate: 0.9603 g (yield: 62%); m.p. 181 °C; IR (ATR cm^{-1}): 3126, 1590, 1491, 1401, 1295, 1122, 1059, 1015, 988, 960, 827, 617, 592, 523. ^1H NMR (400 MHz, DMSO-d_6): δ 7.88 (4H, *d*, $J = 8.9$, Ar—*H*), 7.97 (4H, *d*, $J = 8.9$, Ar—*H*), 8.57 (2H, *s*, Imid-C*H*═C*H*) and 10.37 p.p.m. (1H, *s*, NC*H*N). All other spectroscopic data matched those previously reported. Suitable crystals for X-ray diffraction analysis were grown by layering the DMSO solution with diethyl ether.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2026). **11**, x260253 [https://doi.org/10.1107/S2414314626002531]

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Crystal data

$C_{15}H_{11}Br_2N_2^{+}\cdot BF_4^{-}$
M_r = 465.89
Monoclinic, $C2/c$
a = 9.5407 (2) Å
b = 9.8272 (2) Å
c = 17.0451 (3) Å
β = 102.878 (1)°
V = 1557.92 (5) Å^3
Z = 4

$F(000)$ = 904
D_x = 1.986 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5032 reflections
θ = 2.5–28.2°
μ = 5.25 mm^{-1}
T = 100 K
Block, colourless
0.37 × 0.28 × 0.21 mm

Data collection

Bruker SMART APEXII area detector diffractometer
Radiation source: microfocus sealed X-ray tube, Incoatec Iμs
Mirror optics monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)

$T_{\min}$ = 0.618, $T_{\max}$ = 0.746
9293 measured reflections
1922 independent reflections
1748 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.023
$\theta_{\max}$ = 28.3°, $\theta_{\min}$ = 2.5°
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 13$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.038
S = 1.06
1922 reflections
110 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0133P)^2 + 2.086P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.002
$\Delta\rho_{\max}$ = 0.37 e Å^{-3}
$\Delta\rho_{\min}$ = −0.29 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 (Å^2)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
Br1	0.79285 (2)	0.44748 (2)	0.42461 (2)	0.01694 (5)
F1	0.60495 (11)	1.28959 (10)	0.79615 (6)	0.0298 (2)
F2	0.43907 (13)	1.12447 (11)	0.79918 (7)	0.0379 (3)
N1	0.54845 (13)	0.66867 (12)	0.69843 (7)	0.0130 (2)
C1	0.71272 (15)	0.51725 (16)	0.50861 (9)	0.0153 (3)
C2	0.63143 (15)	0.63529 (15)	0.49678 (9)	0.0150 (3)
H2	0.613229	0.680767	0.446339	0.018*
C3	0.57701 (15)	0.68594 (15)	0.56002 (9)	0.0145 (3)
H3	0.520537	0.766483	0.553292	0.017*
C4	0.60593 (15)	0.61777 (15)	0.63310 (9)	0.0139 (3)
C5	0.500000	0.5896 (2)	0.750000	0.0140 (4)
H5	0.500002	0.492896	0.750001	0.017*
C6	0.53051 (16)	0.80363 (15)	0.71783 (9)	0.0161 (3)
H6	0.556228	0.881331	0.690995	0.019*
C7	0.73926 (16)	0.44820 (16)	0.58138 (9)	0.0175 (3)
H7	0.793608	0.366355	0.587808	0.021*
C8	0.68604 (16)	0.49934 (16)	0.64455 (9)	0.0165 (3)
H8	0.704252	0.453812	0.694975	0.020*
B1	0.500000	1.2063 (3)	0.750000	0.0185 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01930 (8)	0.01754 (8)	0.01556 (8)	−0.00009 (6)	0.00730 (5)	−0.00169 (6)
F1	0.0342 (6)	0.0190 (5)	0.0305 (5)	−0.0001 (4)	−0.0052 (5)	−0.0008 (4)
F2	0.0569 (7)	0.0275 (6)	0.0381 (6)	−0.0040 (5)	0.0292 (6)	0.0094 (5)
N1	0.0148 (6)	0.0119 (6)	0.0123 (6)	−0.0011 (5)	0.0028 (5)	−0.0002 (5)
C1	0.0145 (7)	0.0179 (7)	0.0140 (7)	−0.0039 (6)	0.0045 (5)	−0.0027 (6)
C2	0.0148 (7)	0.0161 (7)	0.0138 (7)	−0.0035 (6)	0.0027 (5)	0.0014 (6)
C3	0.0142 (7)	0.0127 (7)	0.0162 (7)	−0.0015 (5)	0.0024 (6)	0.0008 (5)
C4	0.0137 (6)	0.0157 (7)	0.0129 (6)	−0.0027 (6)	0.0039 (5)	−0.0024 (5)
C5	0.0167 (10)	0.0115 (9)	0.0138 (9)	0.000	0.0031 (8)	0.000
C6	0.0202 (7)	0.0110 (7)	0.0163 (7)	−0.0005 (6)	0.0025 (6)	−0.0002 (5)
C7	0.0174 (7)	0.0166 (7)	0.0184 (7)	0.0024 (6)	0.0038 (6)	0.0002 (6)
C8	0.0185 (7)	0.0167 (7)	0.0138 (7)	0.0006 (6)	0.0030 (6)	0.0023 (6)
B1	0.0280 (13)	0.0122 (11)	0.0173 (11)	0.000	0.0096 (10)	0.000

Geometric parameters (Å, º)

Br1—C1	1.8953 (14)	C3—H3	0.9500
F1—B1	1.3930 (18)	C3—C4	1.387 (2)
F2—B1	1.3799 (18)	C4—C8	1.382 (2)
N1—C4	1.4364 (18)	C5—H5	0.9500
N1—C5	1.3311 (17)	C6—C6$^{\rm i}$	1.351 (3)
N1—C6	1.3867 (19)	C6—H6	0.9500

C1—C2	1.385 (2)	C7—H7	0.9500
C1—C7	1.387 (2)	C7—C8	1.383 (2)
C2—H2	0.9500	C8—H8	0.9500
C2—C3	1.389 (2)		

C5—N1—C4	123.87 (13)	N1^{i}—C5—H5	125.7
C5—N1—C6	108.76 (13)	N1—C6—H6	126.5
C6—N1—C4	127.35 (12)	C6^{i}—C6—N1	106.97 (8)
C2—C1—Br1	120.01 (11)	C6^{i}—C6—H6	126.5
C2—C1—C7	121.65 (14)	C1—C7—H7	120.2
C7—C1—Br1	118.34 (12)	C8—C7—C1	119.54 (14)
C1—C2—H2	120.6	C8—C7—H7	120.2
C1—C2—C3	118.77 (13)	C4—C8—C7	118.90 (14)
C3—C2—H2	120.6	C4—C8—H8	120.5
C2—C3—H3	120.3	C7—C8—H8	120.5
C4—C3—C2	119.35 (14)	F1^{i}—B1—F1	108.01 (18)
C4—C3—H3	120.3	F2—B1—F1	110.28 (7)
C3—C4—N1	119.62 (13)	F2^{i}—B1—F1^{i}	110.28 (7)
C8—C4—N1	118.58 (13)	F2^{i}—B1—F1	109.77 (7)
C8—C4—C3	121.78 (14)	F2—B1—F1^{i}	109.77 (7)
N1^{i}—C5—N1	108.53 (18)	F2^{i}—B1—F2	108.73 (19)
N1—C5—H5	125.7		

Br1—C1—C2—C3	−178.42 (11)	C4—N1—C5—N1^{i}	−178.58 (15)
Br1—C1—C7—C8	177.89 (12)	C4—N1—C6—C6^{i}	178.37 (15)
N1—C4—C8—C7	178.69 (13)	C5—N1—C4—C3	142.28 (12)
C1—C2—C3—C4	0.3 (2)	C5—N1—C4—C8	−36.09 (19)
C1—C7—C8—C4	0.7 (2)	C5—N1—C6—C6^{i}	−0.25 (19)
C2—C1—C7—C8	−1.3 (2)	C6—N1—C4—C3	−36.1 (2)
C2—C3—C4—N1	−179.22 (13)	C6—N1—C4—C8	145.49 (15)
C2—C3—C4—C8	−0.9 (2)	C6—N1—C5—N1^{i}	0.10 (7)
C3—C4—C8—C7	0.4 (2)	C7—C1—C2—C3	0.8 (2)

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···F1^{ii}	0.95	2.29	3.156 (2)	151
C6—H6···F2^{i}	0.95	2.39	3.1854 (19)	140

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