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3-(2-Bromobenzyl)-1-methyl-1*H*-imidazol-3-ium bromide

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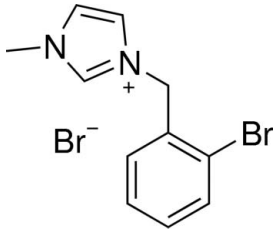
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.013 Å; R factor = 0.064; wR factor = 0.130; data-to-parameter ratio = 15.6.

In the title compound, $C_{11}H_{12}BrN_2^+\cdot Br^-$, the imidazole and phenyl rings are nearly perpendicular, making a dihedral angle of 87.71 (7)°. The crystal structure is stabilized by non-classical intermolecular C—H···Br hydrogen bonds and inversion-related molecules are linked through π–π interactions between the imidazole ring systems [centroid–centroid distance = 3.472 (6) Å].

Related literature

Imidazolium salts are used to obtain transition metal complexes of *N*-heterocyclic carbenes, which have become an important class of catalysts in organometallic chemistry and organic synthesis, see: Marion & Nolan (2008); Herrmann (2002); Qin *et al.* (2006). For related structures, Guo *et al.* (2008); Liu *et al.* (2003).



Experimental

Crystal data

$C_{11}H_{12}BrN_2^+\cdot Br^-$
M_r = 332.05
Orthorhombic, *Pbca*
a = 8.4548 (10) Å
b = 13.9166 (13) Å
c = 20.831 (2) Å
V = 2451.1 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 6.58 mm^{-1}
T = 298 K
0.42 × 0.40 × 0.21 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.169, T_{max} = 0.339
9279 measured reflections
2158 independent reflections
1530 reflections with $I > 2\sigma(I)$
R_{int} = 0.126

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.130
S = 1.19
2158 reflections
138 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···Br2^{i}	0.97	2.86	3.662 (6)	141

Symmetry code: (i) $x+1, y, z$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2011).

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supplementary materials

Acta Cryst. (2011). E**67**, o1568 [**doi:10.1107/S1600536811019842**]

3-(2-Bromobenzyl)-1-methyl-1*H*-imidazol-3-ium bromide

J.-Y. Dong and T.-P. You

Comment

Imidazolium salts or its derivatives are used as ionic liquids, and in many organic transformations. They are used to obtain transition metal complexes of N-heterocyclic carbenes which have become a very important class of catalysts in organometallic chemistry and organic synthesis (Herrmann, 2002, Marion & Nolan, 2008). We here report the crystal structure of the title compound.

Bond lengths and angles in the title molecule (Fig. 1) are within normal ranges. The imidazole and the phenyl ring are nearly perpendicular, with a dihedral angle of 87.71 (2)°.

The molecular structure is stabilized by C—H···Br hydrogen bonds (Table 1). The crystal structure is stabilized by π-π interactions between the imidazole ring systems of the inversion related molecules, with a $Cg1\cdots Cg1^{i}$ distance of 3.472 (6) Å [symmetry code: (i) 1-*x*, -*y*, 1-*z*].

Experimental

1-methyl-1*H*-imidazole (0.615 g, 7.5 mmol) and 1-bromo-2-(bromomethyl)benzene (1.25 g, 5 mmol) in 20 ml of dioxane were refluxed for 12 h. After cooling the solution to room temperature, the mixture was filtered and afforded a colorless solid. Colourless single crystals suitable for X-ray diffraction were obtained by recrystallization from acetonitrile and diethyl ether.

Refinement

H atoms were placed in calculated positions with C—H = 0.95–0.99 Å, and refined in riding mode with U_{iso}(H) = 1.2–1.5U_{eq}(C).

Figures

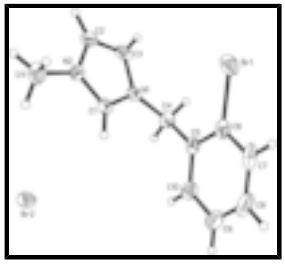

Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

3-(2-Bromobenzyl)-1-methyl-1*H*-imidazol-3-ium bromide

Crystal data

$C_{11}H_{12}BrN_2^+\cdot Br^-$	$D_x = 1.800$ Mg m^{-3}
$M_r = 332.05$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Pbca*	Cell parameters from 992 reflections
$a = 8.4548$ (10) Å	$\theta = 2.6$–$25.2°$
$b = 13.9166$ (13) Å	$\mu = 6.58$ mm^{-1}
$c = 20.831$ (2) Å	$T = 298$ K
$V = 2451.1$ (5) Å^3	Block, colourless
$Z = 8$	0.42 × 0.40 × 0.21 mm
$F(000) = 1296$	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2158 independent reflections
Radiation source: fine-focus sealed tube	1530 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.126$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -10\rightarrow9$
$T_{min} = 0.169$, $T_{max} = 0.339$	$k = -15\rightarrow16$
9279 measured reflections	$l = -15\rightarrow24$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.064$	H-atom parameters constrained
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 1.6882P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.19$	$(\Delta/\sigma)_{max} < 0.001$
2158 reflections	$\Delta\rho_{max} = 0.74$ e Å^{-3}
138 parameters	$\Delta\rho_{min} = -0.65$ e Å^{-3}
0 restraints	Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0051 (4)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations

between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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}
Br1	0.76580 (9)	0.05373 (6)	0.26368 (5)	0.0618 (4)
Br2	0.09361 (7)	0.16571 (5)	0.46240 (4)	0.0464 (3)
N1	0.6110 (5)	0.0692 (4)	0.4078 (3)	0.0320 (14)
N2	0.4228 (6)	−0.0365 (4)	0.4189 (3)	0.0346 (14)
C1	0.4546 (7)	0.0545 (5)	0.4031 (3)	0.0329 (17)
H1	0.3803	0.1002	0.3908	0.039*
C2	0.5601 (8)	−0.0806 (5)	0.4353 (4)	0.0444 (19)
H2	0.5716	−0.1438	0.4490	0.053*
C3	0.6759 (8)	−0.0158 (5)	0.4282 (4)	0.0434 (19)
H3	0.7827	−0.0267	0.4359	0.052*
C4	0.6935 (7)	0.1600 (5)	0.3952 (4)	0.0393 (19)
H4A	0.8059	0.1473	0.3913	0.047*
H4B	0.6785	0.2026	0.4315	0.047*
C5	0.6377 (6)	0.2087 (5)	0.3363 (4)	0.0337 (18)
C6	0.6590 (7)	0.1733 (5)	0.2750 (4)	0.041 (2)
C7	0.6039 (9)	0.2206 (8)	0.2210 (4)	0.061 (2)
H7	0.6185	0.1945	0.1803	0.073*
C8	0.5265 (10)	0.3076 (8)	0.2288 (6)	0.069 (3)
H8	0.4887	0.3404	0.1930	0.083*
C9	0.5056 (9)	0.3454 (7)	0.2885 (6)	0.068 (3)
H9	0.4543	0.4040	0.2933	0.082*
C10	0.5604 (8)	0.2968 (5)	0.3419 (4)	0.049 (2)
H10	0.5454	0.3233	0.3824	0.059*
C11	0.2652 (7)	−0.0794 (6)	0.4187 (4)	0.056 (2)
H11A	0.1878	−0.0308	0.4279	0.084*
H11B	0.2599	−0.1288	0.4508	0.084*
H11C	0.2442	−0.1068	0.3773	0.084*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0619 (5)	0.0619 (6)	0.0615 (8)	−0.0090 (4)	0.0169 (4)	−0.0205 (5)
Br2	0.0390 (4)	0.0502 (5)	0.0500 (7)	0.0086 (3)	−0.0099 (3)	0.0048 (4)
N1	0.030 (3)	0.041 (3)	0.025 (4)	0.007 (3)	−0.002 (2)	0.000 (3)
N2	0.041 (3)	0.035 (3)	0.029 (4)	−0.001 (3)	0.002 (3)	0.000 (3)
C1	0.031 (3)	0.045 (4)	0.023 (5)	0.006 (3)	−0.005 (3)	0.002 (3)
C2	0.049 (4)	0.042 (4)	0.043 (6)	0.010 (4)	0.003 (3)	0.002 (4)

C3	0.041 (4)	0.056 (5)	0.034 (5)	0.020 (4)	−0.003 (3)	0.003 (4)
C4	0.034 (3)	0.045 (4)	0.039 (6)	−0.005 (3)	−0.005 (3)	−0.003 (4)
C5	0.025 (3)	0.039 (4)	0.037 (6)	−0.011 (3)	−0.002 (3)	0.004 (4)
C6	0.032 (3)	0.044 (4)	0.048 (6)	−0.019 (3)	0.004 (3)	−0.002 (4)
C7	0.055 (5)	0.094 (7)	0.033 (6)	−0.031 (5)	0.003 (4)	0.013 (5)
C8	0.051 (5)	0.087 (8)	0.069 (9)	−0.010 (5)	−0.003 (5)	0.045 (6)
C9	0.057 (5)	0.066 (6)	0.081 (9)	0.003 (4)	0.010 (5)	0.030 (6)
C10	0.045 (4)	0.051 (5)	0.052 (7)	−0.005 (3)	0.000 (4)	0.005 (4)
C11	0.045 (4)	0.062 (5)	0.060 (7)	−0.015 (4)	0.001 (4)	−0.005 (5)

Geometric parameters (Å, °)

Br1—C6	1.908 (7)	C5—C6	1.380 (10)
N1—C1	1.342 (7)	C5—C10	1.393 (9)
N1—C3	1.372 (8)	C6—C7	1.385 (11)
N1—C4	1.466 (8)	C7—C8	1.386 (13)
N2—C1	1.336 (9)	C7—H7	0.9300
N2—C2	1.357 (8)	C8—C9	1.362 (14)
N2—C11	1.460 (8)	C8—H8	0.9300
C1—H1	0.9300	C9—C10	1.382 (12)
C2—C3	1.338 (10)	C9—H9	0.9300
C2—H2	0.9300	C10—H10	0.9300
C3—H3	0.9300	C11—H11A	0.9600
C4—C5	1.480 (10)	C11—H11B	0.9600
C4—H4A	0.9700	C11—H11C	0.9600
C4—H4B	0.9700		
C1—N1—C3	106.5 (6)	C10—C5—C4	118.9 (7)
C1—N1—C4	126.0 (5)	C5—C6—C7	122.6 (8)
C3—N1—C4	127.5 (5)	C5—C6—Br1	119.2 (6)
C1—N2—C2	108.6 (5)	C7—C6—Br1	118.2 (7)
C1—N2—C11	124.8 (6)	C6—C7—C8	118.6 (9)
C2—N2—C11	126.6 (6)	C6—C7—H7	120.7
N2—C1—N1	109.0 (5)	C8—C7—H7	120.7
N2—C1—H1	125.5	C9—C8—C7	120.4 (9)
N1—C1—H1	125.5	C9—C8—H8	119.8
C3—C2—N2	107.1 (6)	C7—C8—H8	119.8
C3—C2—H2	126.5	C8—C9—C10	120.2 (9)
N2—C2—H2	126.5	C8—C9—H9	119.9
C2—C3—N1	108.8 (6)	C10—C9—H9	119.9
C2—C3—H3	125.6	C9—C10—C5	121.3 (9)
N1—C3—H3	125.6	C9—C10—H10	119.3
N1—C4—C5	113.1 (5)	C5—C10—H10	119.3
N1—C4—H4A	109.0	N2—C11—H11A	109.5
C5—C4—H4A	109.0	N2—C11—H11B	109.5
N1—C4—H4B	109.0	H11A—C11—H11B	109.5
C5—C4—H4B	109.0	N2—C11—H11C	109.5
H4A—C4—H4B	107.8	H11A—C11—H11C	109.5
C6—C5—C10	116.9 (7)	H11B—C11—H11C	109.5
C6—C5—C4	124.2 (7)		

C2—N2—C1—N1	1.3 (8)	N1—C4—C5—C10	114.2 (7)
C11—N2—C1—N1	−179.2 (7)	C10—C5—C6—C7	−1.5 (9)
C3—N1—C1—N2	−0.9 (8)	C4—C5—C6—C7	179.4 (6)
C4—N1—C1—N2	−179.3 (6)	C10—C5—C6—Br1	179.4 (4)
C1—N2—C2—C3	−1.1 (8)	C4—C5—C6—Br1	0.3 (8)
C11—N2—C2—C3	179.4 (7)	C5—C6—C7—C8	1.0 (10)
N2—C2—C3—N1	0.5 (9)	Br1—C6—C7—C8	−179.8 (5)
C1—N1—C3—C2	0.3 (8)	C6—C7—C8—C9	0.0 (11)
C4—N1—C3—C2	178.6 (7)	C7—C8—C9—C10	−0.5 (12)
C1—N1—C4—C5	−44.1 (9)	C8—C9—C10—C5	0.0 (11)
C3—N1—C4—C5	137.9 (7)	C6—C5—C10—C9	1.0 (10)
N1—C4—C5—C6	−66.7 (8)	C4—C5—C10—C9	−179.9 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4A···Br2^{i}	0.97	2.86	3.662 (6)	141

Symmetry codes: (i) *x*+1, *y*, *z*.

Fig. 1