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3,3′-Dibenzyl-1,1′-ethylenediimidazolium dibromide

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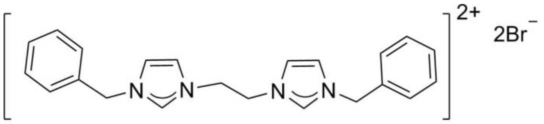
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.074; data-to-parameter ratio = 20.0.

In the title compound, $C_{22}H_{24}N_4^{2+}\cdot 2Br^-$, the imidazolium dication is located on a crystallographic inversion center. The imidazole and benzene rings make a dihedral angle of 73.1 (9)°. In the crystal, non-classical intermolecular C—H⋯Br hydrogen bonds link the ion pairs into a two-dimensional network.

Related literature

For related structures of bis(imidazolium) salts, see: Baker *et al.* (2002); Lee *et al.* (2004, 2007, 2008); Jin *et al.* (2007); Lee & Lu (2008); Paulose *et al.* (2008) and of methylene-linked bis(imidazolium) salts, see: Cheng *et al.* (2006); Lee & Chiu (2004); Lee *et al.* (2004).



Experimental

Crystal data

$C_{22}H_{24}N_4^{2+}\cdot 2Br^-$	V = 1054.76 (8) Å^3
M_r = 504.27	Z = 2
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 16.4674 (8) Å	μ = 3.86 mm^{-1}
b = 5.2099 (2) Å	T = 150 K
c = 12.3736 (6) Å	0.25 × 0.20 × 0.20 mm
β = 96.495 (3)°	

Data collection

Bruker SMART APEXII diffractometer	10232 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	2542 independent reflections
T_{min} = 0.446, T_{max} = 0.513	1915 reflections with $I > 2\sigma$
	R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031	127 parameters
$wR(F^2)$ = 0.074	H-atom parameters constrained
S = 1.03	$\Delta\rho_{max}$ = 0.49 e Å^{-3}
2542 reflections	$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C1—H1⋯Br1^{i}	0.95	2.86	3.663 (2)	143
C3—H3⋯Br1^{ii}	0.95	2.77	3.683 (2)	162
C4—H4B⋯Br1^{i}	0.99	2.83	3.661 (3)	142

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

Data collection: *APEX2* (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: *DIAMOND* (Brandenburg, 2006).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2353).

References

Baker, R. J., Cole, M. L., Jones, C. & Mahon, M. F. (2002). *J. Chem. Soc. Dalton Trans.* pp. 1992–1996.
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cheng, P.-Y., Chen, C.-Y. & Lee, H. M. (2006). *Acta Cryst.* E**62**, o5850–o5851.
Jin, H.-S., Wang, H.-J., Zhang, Y., Zuo, Y.-J. & Zhong, C.-M. (2007). *Acta Cryst.* E**63**, o1880–o1881.
Lee, H. M., Chen, C.-Y., Chen, W.-L. & Lin, H.-C. (2007). *Acta Cryst.* E**63**, o315–o316.
Lee, H. M. & Chiu, P.-L. (2004). *Acta Cryst.* E**60**, o1385-o1386.
Lee, H. M. & Lu, C.-Y. (2008). *Acta Cryst.* E**64**, o2086.
Lee, H. M., Lu, C. Y., Chen, C. Y., Chen, W. L., Lin, H. C., Chiu, P. L. & Cheng, P. Y. (2004). *Tetrahedron*, **60**, 5807–5825.
Lee, H. M., Lu, C.-Y. & Cheng, P.-Y. (2008). *Acta Cryst.* E**64**, m1028.
Paulose, T. A. P., Olson, J. A., Quail, J. W. & Foley, S. R. (2008). *J. Organomet. Chem*, **693**, 3405–3410.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

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3,3′-Dibenzyl-1,1′-ethylenediimidazolium dibromide

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S1. Comment

The title compound is a precursor to the formation of bidentate *N*-heterocyclic carbene ligand (Lee *et al.* 2004). It can be easily prepared by the reaction of 1,2-dibromoethane and 1-benzylimidazole in tetrahydrofuran (Lee *et al.* 2004).

The dication is located on a crystallographic inversion center. The non-classical intermolecular hydrogen bonds of the type C—H···Br link the imidazolium dications and bromide anions into a two dimensional hydrogen bonded network.

Ethylene-linked bis(imidazolium) salts similar to the title compound were reported by us (Lee *et al.*, 2004; Lee *et al.* 2007; Lee & Lu (2008); Lee *et al.* 2008) and others (Baker *et al.* 2002; Jin *et al.* 2007; Paulose *et al.* 2008). We also published crystal structures of relevant methylene-linked bis(imidazolium) salts (Lee *et al.*, 2004; Lee & Chiu, 2004; Cheng *et al.* 2006).

S2. Experimental

The compound was prepared according to the literature procedure (Lee *et al.*, 2004). Suitable crystals were obtained by slow diffusion of diethyl ether into a DMF solution of the compound at room temperature.

S3. Refinement

All the hydrogen atoms were discerned in the difference Fourier map, nevertheless, all the H atoms were positioned geometrically and refined as riding atoms, with C_{aryl}—H = 0.95, $C_{methylene}$ —H = 0.99 Å while $U_{iso}(H) = 1.2U_{eq}(C)$ for all the H atoms.

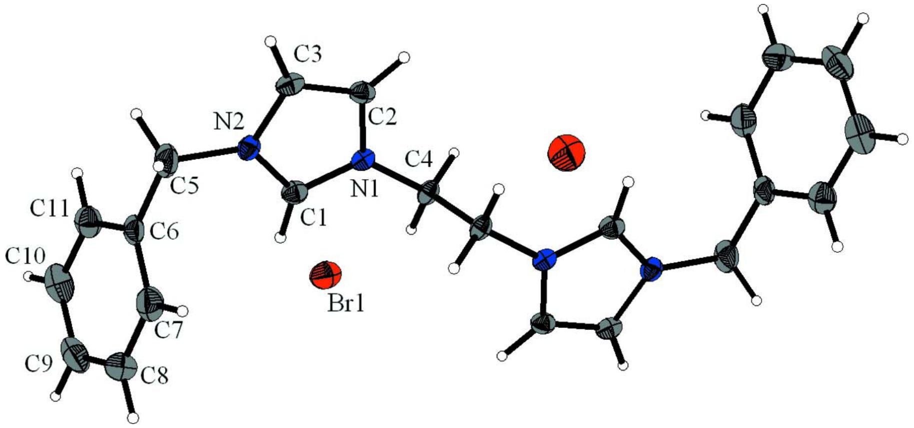

Figure 1

The structure of the title compound, showing 50% probability displacement ellipsoids for the non-hydrogen atoms. The H atoms are depicted by circles of an arbitrary radius. The unlabelled atoms of the imidazolium cation and the bromide anion are related to the labelled ones by 1 - *x*, -*y*, 1 - *z*.

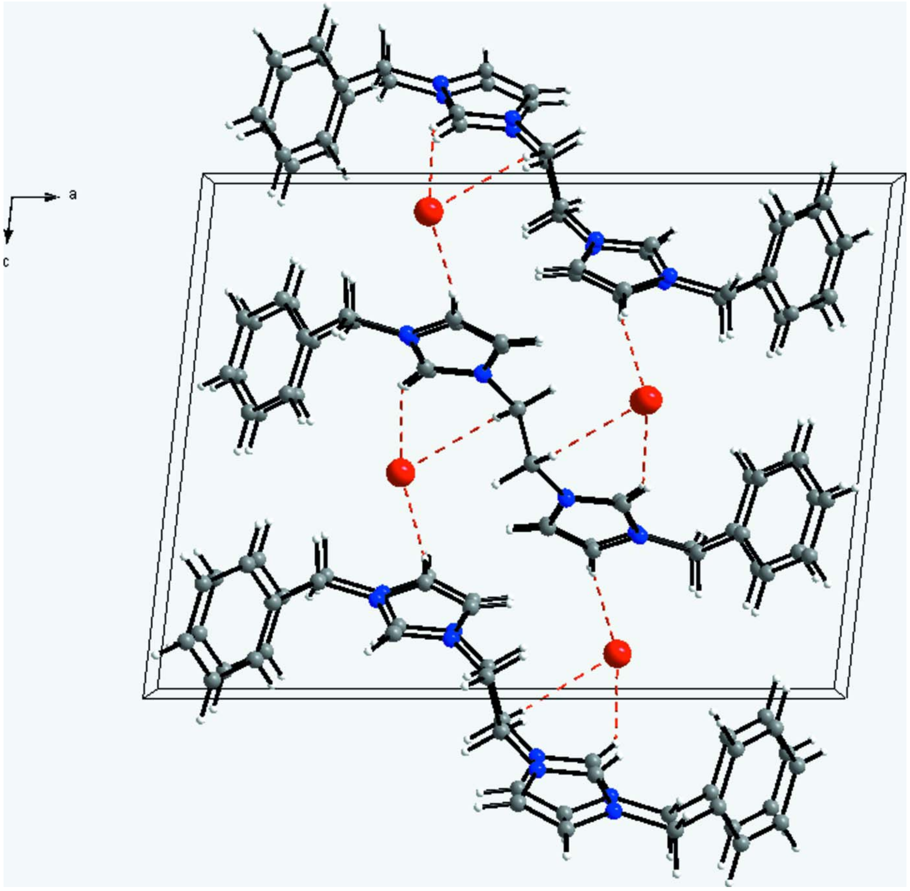

Figure 2

A view of the crystal packing along the *b* axis. Hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{22}H_{24}N_4^{2+}\cdot 2Br^-$
$M_r = 504.27$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 16.4674$ (8) Å
$b = 5.2099$ (2) Å
$c = 12.3736$ (6) Å
$\beta = 96.495$ (3)°
$V = 1054.76$ (8) Å^3
$Z = 2$

$F(000) = 508$
$D_x = 1.588$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2242 reflections
$\theta = 2.5$–24.5°
$\mu = 3.86$ mm^{-1}
$T = 150$ K
Block, colorless
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.446$, $T_{max} = 0.513$

10232 measured reflections
2542 independent reflections
1915 reflections with $I > 2\sigma$
$R_{int} = 0.047$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.5°$
$h = -21 \rightarrow 21$
$k = -6 \rightarrow 6$
$l = -16 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.074$
$S = 1.03$
2542 reflections
127 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
$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 0.006P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

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	0.326856 (16)	0.58076 (5)	0.570787 (19)	0.02456 (10)
C1	0.34814 (15)	0.0860 (5)	0.37001 (19)	0.0191 (5)
H1	0.3171	−0.0415	0.4018	0.023*
C2	0.45155 (15)	0.3145 (5)	0.32355 (19)	0.0186 (5)
H2	0.5056	0.3725	0.3176	0.022*
C3	0.38199 (15)	0.4239 (5)	0.27857 (19)	0.0196 (5)
H3	0.3777	0.5737	0.2345	0.024*
C4	0.48543 (14)	−0.0683 (4)	0.44729 (18)	0.0173 (5)
H4A	0.5327	−0.1128	0.4082	0.021*
H4B	0.4569	−0.2290	0.4628	0.021*
C5	0.23178 (16)	0.3432 (5)	0.2752 (2)	0.0300 (7)
H5A	0.2227	0.3566	0.1949	0.036*
H5B	0.2199	0.5131	0.3056	0.036*
C6	0.17344 (15)	0.1494 (5)	0.3122 (2)	0.0230 (6)
C7	0.15780 (16)	0.1430 (6)	0.4197 (2)	0.0324 (7)
H7	0.1842	0.2621	0.4701	0.039*
C8	0.10409 (18)	−0.0349 (6)	0.4545 (3)	0.0381 (8)
H8	0.0944	−0.0402	0.5287	0.046*
C9	0.06422 (16)	−0.2064 (6)	0.3799 (3)	0.0380 (8)
H9	0.0271	−0.3289	0.4031	0.046*
C10	0.07858 (17)	−0.1982 (6)	0.2731 (3)	0.0350 (7)
H10	0.0508	−0.3134	0.2221	0.042*
C11	0.13354 (16)	−0.0224 (5)	0.2392 (2)	0.0281 (6)
H11	0.1439	−0.0199	0.1652	0.034*
N1	0.42965 (12)	0.1019 (4)	0.37997 (15)	0.0166 (4)

N2	0.31810 (11)	0.2793 (4)	0.30799 (15)	0.0178 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03007 (16)	0.02334 (15)	0.02017 (15)	−0.00608 (12)	0.00241 (10)	−0.00064 (12)
C1	0.0225 (13)	0.0160 (13)	0.0189 (12)	−0.0020 (10)	0.0028 (10)	0.0006 (11)
C2	0.0212 (14)	0.0178 (12)	0.0172 (12)	−0.0042 (10)	0.0035 (10)	−0.0002 (10)
C3	0.0263 (14)	0.0179 (13)	0.0148 (12)	−0.0014 (11)	0.0030 (10)	0.0003 (11)
C4	0.0188 (12)	0.0161 (12)	0.0162 (12)	0.0047 (10)	−0.0014 (9)	0.0011 (10)
C5	0.0204 (14)	0.0286 (15)	0.0395 (17)	0.0048 (11)	−0.0040 (12)	0.0103 (12)
C6	0.0147 (13)	0.0236 (14)	0.0298 (15)	0.0041 (10)	−0.0025 (11)	0.0049 (11)
C7	0.0248 (16)	0.0372 (17)	0.0338 (17)	−0.0022 (11)	−0.0022 (13)	−0.0028 (13)
C8	0.0304 (17)	0.053 (2)	0.0318 (17)	0.0014 (14)	0.0078 (13)	0.0109 (15)
C9	0.0200 (15)	0.0320 (17)	0.062 (2)	−0.0003 (12)	0.0056 (14)	0.0132 (16)
C10	0.0263 (16)	0.0279 (16)	0.050 (2)	0.0014 (12)	0.0011 (14)	−0.0091 (14)
C11	0.0241 (15)	0.0290 (15)	0.0310 (16)	0.0058 (11)	0.0023 (12)	−0.0036 (12)
N1	0.0205 (11)	0.0154 (10)	0.0135 (10)	0.0004 (8)	0.0012 (8)	0.0004 (8)
N2	0.0193 (11)	0.0155 (11)	0.0179 (11)	0.0009 (8)	−0.0008 (8)	0.0020 (9)

Geometric parameters (Å, º)

C1—N2	1.328 (3)	C5—H5A	0.9900
C1—N1	1.336 (3)	C5—H5B	0.9900
C1—H1	0.9500	C6—C7	1.384 (4)
C2—C3	1.343 (3)	C6—C11	1.384 (4)
C2—N1	1.379 (3)	C7—C8	1.383 (4)
C2—H2	0.9500	C7—H7	0.9500
C3—N2	1.376 (3)	C8—C9	1.394 (4)
C3—H3	0.9500	C8—H8	0.9500
C4—N1	1.467 (3)	C9—C10	1.369 (4)
C4—C4$^{\mathrm{i}}$	1.515 (4)	C9—H9	0.9500
C4—H4A	0.9900	C10—C11	1.386 (4)
C4—H4B	0.9900	C10—H10	0.9500
C5—N2	1.472 (3)	C11—H11	0.9500
C5—C6	1.501 (4)		

N2—C1—N1	108.1 (2)	C11—C6—C5	120.6 (3)
N2—C1—H1	125.9	C6—C7—C8	120.7 (3)
N1—C1—H1	125.9	C6—C7—H7	119.7
C3—C2—N1	106.9 (2)	C8—C7—H7	119.7
C3—C2—H2	126.5	C7—C8—C9	119.6 (3)
N1—C2—H2	126.5	C7—C8—H8	120.2
C2—C3—N2	107.5 (2)	C9—C8—H8	120.2
C2—C3—H3	126.3	C10—C9—C8	119.9 (3)
N2—C3—H3	126.3	C10—C9—H9	120.0
N1—C4—C4$^{\mathrm{i}}$	108.8 (2)	C8—C9—H9	120.0
N1—C4—H4A	109.9	C9—C10—C11	120.2 (3)

C4^{i}—C4—H4A	109.9	C9—C10—H10	119.9
N1—C4—H4B	109.9	C11—C10—H10	119.9
C4^{i}—C4—H4B	109.9	C6—C11—C10	120.6 (3)
H4A—C4—H4B	108.3	C6—C11—H11	119.7
N2—C5—C6	113.3 (2)	C10—C11—H11	119.7
N2—C5—H5A	108.9	C1—N1—C2	108.7 (2)
C6—C5—H5A	108.9	C1—N1—C4	125.0 (2)
N2—C5—H5B	108.9	C2—N1—C4	126.2 (2)
C6—C5—H5B	108.9	C1—N2—C3	108.8 (2)
H5A—C5—H5B	107.7	C1—N2—C5	128.0 (2)
C7—C6—C11	119.1 (3)	C3—N2—C5	123.1 (2)
C7—C6—C5	120.3 (2)		

N1—C2—C3—N2	0.3 (3)	N2—C1—N1—C4	176.4 (2)
N2—C5—C6—C7	76.1 (3)	C3—C2—N1—C1	−0.7 (3)
N2—C5—C6—C11	−105.0 (3)	C3—C2—N1—C4	−176.2 (2)
C11—C6—C7—C8	1.0 (4)	C4^{i}—C4—N1—C1	−100.5 (3)
C5—C6—C7—C8	180.0 (3)	C4^{i}—C4—N1—C2	74.3 (3)
C6—C7—C8—C9	−1.2 (4)	N1—C1—N2—C3	−0.7 (3)
C7—C8—C9—C10	0.2 (4)	N1—C1—N2—C5	−179.3 (2)
C8—C9—C10—C11	1.0 (4)	C2—C3—N2—C1	0.2 (3)
C7—C6—C11—C10	0.1 (4)	C2—C3—N2—C5	178.9 (2)
C5—C6—C11—C10	−178.8 (2)	C6—C5—N2—C1	−4.6 (4)
C9—C10—C11—C6	−1.1 (4)	C6—C5—N2—C3	176.9 (2)
N2—C1—N1—C2	0.9 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···Br1^{ii}	0.95	2.86	3.663 (2)	143
C3—H3···Br1^{iii}	0.95	2.77	3.683 (2)	162
C4—H4*B*···Br1^{ii}	0.99	2.83	3.661 (3)	142

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