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**1,1'-Bis(3-methoxybenzyl)-3,3'-methylene-  
diimidazolium dibromide**

The structure of the title compound,  $C_{23}H_{25}N_4O_2^{2+} \cdot 2Br^-$ , has been determined at 294 K. The central C atom of the cation is located on a crystallographic twofold rotation axis. Non-classical intermolecular hydrogen bonds of the types C—H $\cdots$ Br and C—H $\cdots$ O are present in the crystal structure.

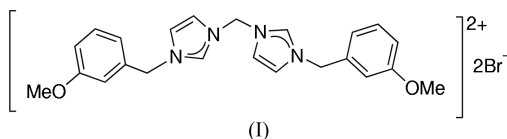
Received 7 July 2004  
Accepted 16 July 2004  
Online 24 July 2004**Key indicators**

Single-crystal X-ray study  
 $T = 294$  K  
 Mean  $\sigma(C-C) = 0.003$  Å  
 R factor = 0.029  
 wR factor = 0.077  
 Data-to-parameter ratio = 19.7

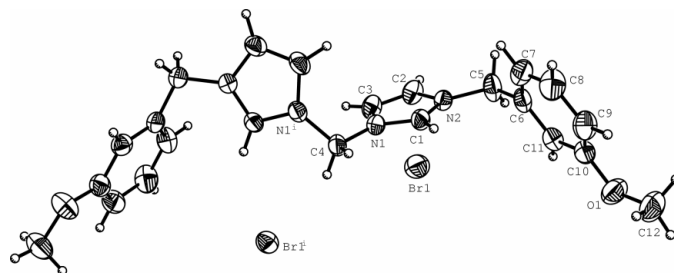
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

**Comment**

N-Heterocyclic carbene (NHC) ligands have been shown to have wide applicability in coordination chemistry and catalysis. Current research efforts are devoted to the discovery of efficient metal NHC catalysts. NHC ligands are generally accessible *via* the deprotonation of imidazolium salts. The preparation of chelating bis(NHC) ligands are also receiving much attention, since they can provide extra air- and moisture stability for the metal centers. For example, chelating palladium complexes of bis(NHC) carbenes have been found to be efficient catalysts in C—C coupling reactions (Herrmann *et al.*, 1998; Zhang & Trudell, 2000). Several bis(imidazolium) halides, as bis(NHC) ligand precursors, have been synthesized and structurally characterized by us (Lee *et al.*, 2004). We report here the structure of 1,1'-bis(3-methoxybenzyl)-3,3'-methylenediimidazolium dibromide, (I). The structure of the 4-methoxy isomer, (II), has been reported previously (Lee *et al.*, 2004).



The title compound, (I), crystallizes in the monoclinic space group  $C2/c$  with one-half cation and one bromide anion in the asymmetric unit. The central C atom of the cation is located on a crystallographic twofold rotation axis, parallel to the  $b$  axis (Fig. 1) The dihedral angle between the two methylene-linked

**Figure 1**

The structure of (I), showing 50% displacement ellipsoids for non-H atoms. [Symmetry code: (i)  $-x, y, \frac{1}{2} - z$ .]

imidazole rings is 78.02 (7)°. The molecular dimensions of (I) are similar to those in (II).

Non-classical hydrogen bonds exist, involving the methoxy groups of adjacent molecules (Table 1), such that the structure of (I) consists of chains of bis(imidazolium) cations running along the [100] direction. These chains are linked by C—H...Br intermolecular hydrogen bonds (Fig. 2).

### Experimental

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

#### Crystal data

$C_{23}H_{25}N_4O_2^{2+} \cdot 2Br^-$	$D_x = 1.543 \text{ Mg m}^{-3}$
$M_r = 549.29$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 786 reflections
$a = 37.557 (5) \text{ \AA}$	$\theta = 3.5\text{--}26.8^\circ$
$b = 5.3553 (6) \text{ \AA}$	$\mu = 3.46 \text{ mm}^{-1}$
$c = 12.3209 (15) \text{ \AA}$	$T = 294 (2) \text{ K}$
$\beta = 107.412 (4)^\circ$	Block, colorless
$V = 2364.6 (5) \text{ \AA}^3$	$0.35 \times 0.20 \times 0.15 \text{ mm}$
$Z = 4$	

#### Data collection

Bruker SMART 1000 diffractometer	2782 independent reflections
$\omega$ scans	2167 reflections with $I > 2\sigma$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$R_{int} = 0.025$
$T_{min} = 0.359, T_{max} = 0.594$	$\theta_{max} = 28.0^\circ$
7332 measured reflections	$h = -41 \rightarrow 49$
	$k = -7 \rightarrow 6$
	$l = -16 \rightarrow 16$

#### Refinement

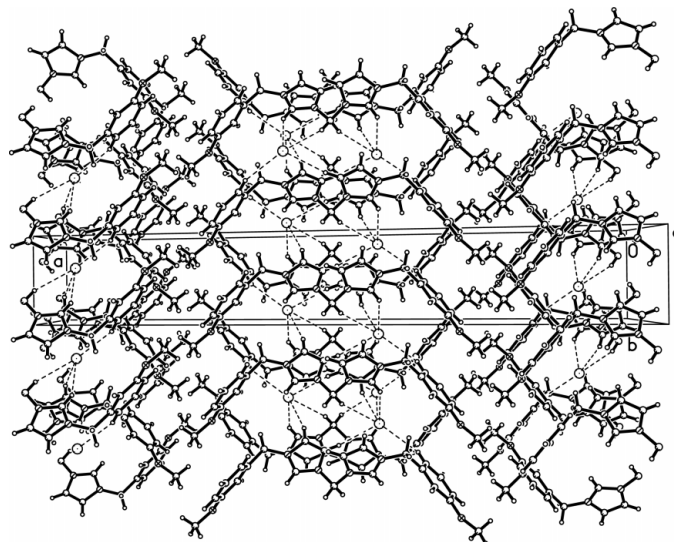
Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 1.0229P]$
$R[F^2 > 2\sigma(F^2)] = 0.029$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.077$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.51 \text{ e \AA}^{-3}$
2782 reflections	$\Delta\rho_{min} = -0.22 \text{ e \AA}^{-3}$
141 parameters	
H-atom parameters constrained	

**Table 1**

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C1—H1A...Br1	0.93	2.80	3.614 (2)	147
C2—H2A...Br1 <sup>i</sup>	0.93	2.72	3.614 (2)	162
C3—H3A...Br1 <sup>ii</sup>	0.93	2.75	3.652 (2)	164
C4—H4A...Br1	0.94	2.83	3.7274 (17)	160
C7—H7A...Br1 <sup>iii</sup>	0.93	2.92	3.793 (3)	156
C8—H8A...O1 <sup>iv</sup>	0.93	2.68	3.515 (3)	150
C12—H12A...O1 <sup>v</sup>	0.96	2.67	3.533 (3)	150

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



**Figure 2**

A view of the packing of (I), approximately along the  $c$  axis. Hydrogen bonds are indicated by dashed lines.

All H atoms were positioned geometrically and refined in the riding-model approximation, with  $U_{iso}(H) = 1.5U_{eq}(C)$  for methyl H atoms and  $1.2U_{eq}(C)$  for all other H atoms. C—H distances are in the range 0.93–0.97 Å.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1998); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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