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# 4,5-Dibromo-1-methyl-1*H*-imidazole

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**Key indicators**

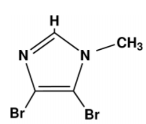
Single-crystal X-ray study
*T* = 174 K
Mean *σ*(C–C) = 0.006 Å
*R* factor = 0.032
*wR* factor = 0.080
Data-to-parameter ratio = 20.1

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

The title compound, $C_4H_4Br_2N_2$, crystallizes with two molecules in the asymmetric unit. Each molecule forms stacks with its own kind, the stacks being approximately orthogonal to each other. Both Br atoms in molecule 1 form Lewis acid–base interactions with N atoms in molecule 2, with Br···N distances of 3.078 (4) and 3.264 (4) Å.

## Comment

In the course of work intended to continue a study of copper(I) cyanide complexes with imidazoles (Stocker *et al.*, 2000), we have determined the structure of the title compound, (I).



(I)

There are two molecules in the asymmetric unit. The anisotropic displacement ellipsoids and atom labelling are shown in Fig. 1. The bond lengths and angles in the two molecules agree within experimental error. They also agree with the values in unsubstituted imidazole (Craven *et al.*, 1977).

Both independent molecules form stacks with their own kind. Views down the stacks are shown in Fig. 2. The stacks of molecule 1 are parallel to the *b* axis, those of molecule 2 are parallel to the *a* axis.

In both stacks, adjacent molecules are related by inversion centers. In stack 1, the upper molecule and the central one each have a Br atom above or below the ring in the next molecule at the perpendicular distance of 3.655 (2) Å. The lower and central molecules have the rings overlapping at a distance of 3.285 (2) Å. In stack 2, the overlaps on both sides are similar to the Br–ring overlaps in stack 1, with distances of 3.626 (2) and 3.754 (2) Å. In each of the three Br–ring overlaps, there are intermolecular H···Br contacts of 3.10 Å or less. The metric details are given in Table 1.

Just as the two stacks are significantly different, the interactions between the two kinds of stacks are also significantly different. There is a C—H···N interaction between molecules in adjacent stacks of molecule 1, but no similar interaction between stacks of molecule 2. Both Br atoms in molecule 1 interact with N atoms in molecule 2 with short Br···N distances (see Fig. 3). There are no Br···N interactions involving the Br atoms in molecule 2. There are also no Br···Br contacts closer than 3.6 Å in the entire structure. The metric details of the interactions are given in Table 1.

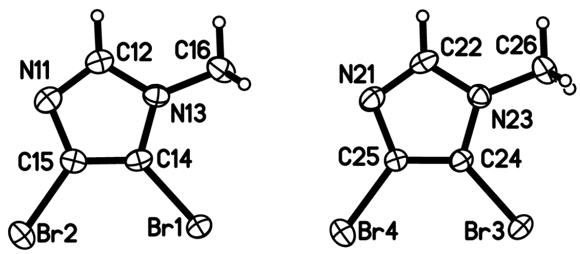



**Figure 1**
The two independent $C_4H_6Br_2N_2$ molecules. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown with arbitrary radii.

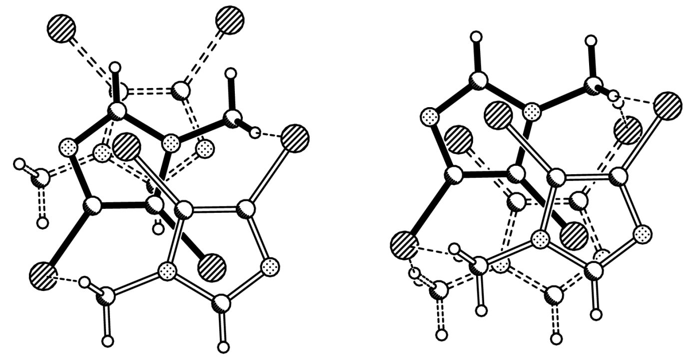


**Figure 2**
The $\pi$–$\pi$ overlap between the molecules, viewed normal to the plane of the molecules. Left: molecule 1; right: molecule 2. The solid bonds define the central molecule in each case, the open bonds the molecule above, the dashed bonds the molecule below. The dashed lines show the H···Br contacts at 3.1 Å or less.

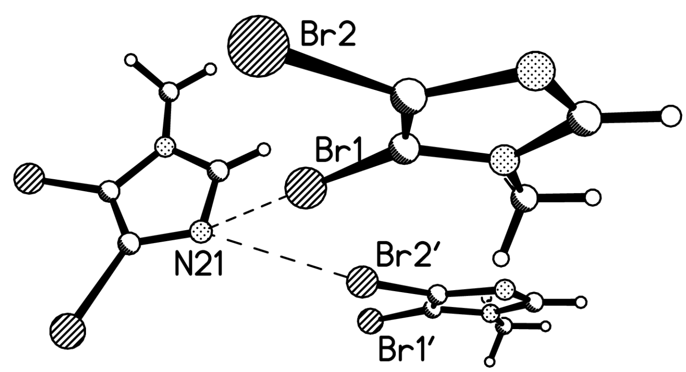



**Figure 3**
View showing the Br···N interactions.

## Experimental

The title compound has been prepared previously by dibromination of 1-methyl-1*H*-imidazole with bromine in chloroform at 278–283 K in 0.5% yield (as the picrate; along with 13% of the 2,4,5-tribromo compound; Balaban & Pyman, 1924), or with *N*-bromosuccinimide in refluxing $CHCl_3$ in 25–40% yield (El Borai *et al.*, 1981). We used a modification of the latter procedure, with *N*-bromosuccinimide in $CH_2Cl_2$. Addition of 3 drops of hydrogen peroxide and irradiation with a tungsten lamp produced a vigorous exothermic reaction, with foaming, which gave the desired product as colorless needles, m.p. 352–353 K; literature: colorless, m.p. 351–352 (Sonn *et al.*, 1924), 352–353 (Balaban & Pyman, 1924), 353 (El Borai *et al.*, 1981), 353–354 (Boulton & Coller, 1974), 354 K (Katritzky *et al.*, 1989); IR (KBr) $cm^{-1}$ 3110 (*w*) and 3092 (*w*, 2-CH), 2943 (*w*, 1-$CH_3$), 1490 (*s*), 1248 (*ms*), 1101 (*ms*), 958 (*s*); $^1$H NMR ($CDCl_3$): $\delta$ 7.45 (*s*, 0.8H, 2-H), 3.62 (*s*, 3H, 1-$CH_3$); $^{13}$C NMR ($CDCl_3$): $\delta$ 137.5 (2-CH), 116.8 (5-C), 104.4(4-C), 34.1 (1-$CH_3$). The literature $^1$H NMR (El Borai *et al.*, 1981; Boulton & Coller, 1974; Katritzky *et al.*, 1989; O'Connell *et al.*, 1988) and $^{13}$C NMR (Katritzky *et al.*, 1989) data are in reasonable agreement with those for (I).

*Crystal data*

$C_4H_4Br_2N_2$
$M_r = 239.91$
Triclinic, $P\bar{1}$
$a = 7.449$ (2) Å
$b = 7.537$ (2) Å
$c = 12.403$ (3) Å
$\alpha = 73.47$ (3)°
$\beta = 79.92$ (3)°
$\gamma = 85.45$ (3)°
$V = 656.9$ (3) Å$^3$
$Z = 4$
$D_x = 2.426$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1490 reflections
$\theta = 2.8$–27.4°
$\mu = 12.23$ mm$^{-1}$
$T = 174$ (2) K
Prism, colorless
0.20 × 0.15 × 0.07 mm

*Data collection*

Siemens SMART area-detector diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)
$T_{min} = 0.12$, $T_{max} = 0.42$
6725 measured reflections
2962 independent reflections
2615 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5°$
$h = -9 \rightarrow 9$
$k = -9 \rightarrow 9$
$l = -16 \rightarrow 15$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.080$
$S = 1.08$
2962 reflections
147 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 1.41P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.82$ e Å$^{-3}$
$\Delta\rho_{min} = -0.72$ e Å$^{-3}$

**Table 1**
Distances and angles (Å, °) in the C—$X$···$Y$—C contacts.

| $X$ | $Y$ | C—H | C—$X$···$Y$ | $X$···$Y$ | $X$···$Y$—C | C(H)···$X$ |
|---|---|---|---|---|---|---|
| H16*A* | Br2$^{i}$ | 0.98 | 158 | 3.04 | 82 | 3.969 (4) |
| H26*B* | Br4$^{ii}$ | 0.98 | 148 | 3.10 | 98 | 3.958 (4) |
| H26*C* | Br4$^{iii}$ | 0.98 | 171 | 3.02 | 80 | 3.986 (4) |
| H16*C* | N11$^{iv}$ | 0.98 | 127 | 2.70 | 114 | 3.383 (5) |
| Br1 | N21$^{i}$ | – | 173.9 (4) | 3.078 (4) | 94.2 (4), 137.5 (4) | – |
| Br2 | N21$^{v}$ | – | 166.5 (4) | 3.264 (4) | 87.9 (4), 143.6 (4) | – |

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1-x, 1-y, -z$; (iii) $-x, 1-y, -z$; (iv) $1-x, -y, 1-z$; (v) $-x, 1-y, 1-z$.

All of the peaks higher than 0.4 e Å$^{-3}$ in the final difference Fourier map lie about 1 Å from a Br atom. The methyl H atoms were included at idealized positions, with the methyl groups allowed to rotate around the C—C bonds.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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