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Bis(2-methylimidazol-1-yl)methane

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Key indicators

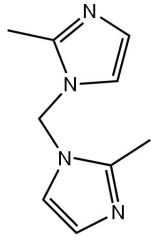
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.068
wR factor = 0.169
Data-to-parameter ratio = 13.5

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

In the title compound, $C_9H_{12}N_4$, the asymmetric unit contains one half-molecule. The C atom of the bridging methylene group lies on a twofold rotation axis. The dihedral angle between the symmetry-related imidazole rings is 88.1 (2)°.

Comment

Polyazolylmethanes have attracted considerable attention in the fields of biochemistry (Sorrell & Borovik, 1987), materials chemistry (Muller *et al.*, 2001), heterocyclic chemistry (Juliá *et al.*, 1982) and coordination chemistry (Effendy *et al.*, 2003). Although many structures of their metal complexes have been reported, there are only a few reports on the structures of the ligands themselves.



(I)

The title compound, (I) (Fig. 1), was prepared by using the phase-transfer organic synthesis method (Juliá *et al.*, 1984). The asymmetric unit consists of one half-molecule. The C atom of the bridging methylene group lies on a twofold rotation axis.

The back donation of the lone pair of electrons of atom N1 may affect the C—N bond lengths and C—N—C bond angles. The dihedral angle between the symmetry-related imidazole rings is 88.1 (2)°.

Experimental

The title molecule was synthesized by modifying the literature method of Diez-Barra *et al.* (1993) and was identified by ^{1}H NMR [300 MHz, $CDCl_3$: δ 6.87 (2H, *s*), 6.77 (2H, *s*), 5.77 (2H, *s*), 2.37 (6H, *s*)] and ^{13}C NMR (δ 144.8, 128.9, 119.1, 55.7, 13.7). It was crystallized from a chloroform–methanol (5:1) mixture by slow evaporation (yield: 50 mg, 72%, m.p. 447–449 K).

Crystal data

$C_9H_{12}N_4$
M_r = 176.23
Monoclinic, $C2/c$
a = 12.371 (2) Å
b = 8.6873 (16) Å
c = 9.9175 (18) Å
β = 120.599 (3)°
V = 917.4 (3) Å^3
Z = 4
D_x = 1.276 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 958 reflections
θ = 6.1–50.4°
μ = 0.08 mm^{-1}
T = 298 (2) K
Block, colorless
0.52 × 0.24 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer	826 independent reflections
φ and ω scans	668 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.018$
$T_{min} = 0.976$, $T_{max} = 0.982$	$\theta_{max} = 25.3^\circ$
2281 measured reflections	$h = -12 \rightarrow 14$
	$k = -10 \rightarrow 8$
	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0801P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.068$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.169$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.31$ e Å^{-3}
826 reflections	Extinction correction: *SHELXL97*
61 parameters	Extinction coefficient: 0.022 (6)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N1—C3	1.362 (2)	N2—C3	1.309 (3)
N1—C1	1.374 (3)	N2—C2	1.368 (3)
N1—C4	1.445 (2)	C3—C5	1.483 (3)
C1—C2	1.341 (3)		
C3—N1—C1	107.29 (15)	C1—C2—N2	111.0 (2)
C3—N1—C4	127.18 (14)	N2—C3—N1	110.62 (16)
C1—N1—C4	125.46 (14)	N2—C3—C5	125.28 (17)
C2—C1—N1	105.35 (17)	N1—C3—C5	124.09 (18)
C3—N2—C2	105.69 (15)	N1—C4—N1^{i}	112.4 (2)
C3—N1—C1—C2	−0.3 (2)	C2—N2—C3—N1	−0.1 (2)
N1—C1—C2—N2	0.2 (2)	C1—N1—C3—N2	0.3 (2)
C3—N2—C2—C1	−0.1 (2)		

Symmetry code: (i) $1 - x, y, \frac{1}{2} - z$.

H atoms were positioned geometrically at distances of 0.93 (CH), 0.97 (CH_2) and 0.96 Å (CH_3) from the parent C atoms; a riding model was used during the refinement process. The U_{iso}(H) values were constrained to be 1.2 (1.5 for methyl) times U_{eq} of the carrier atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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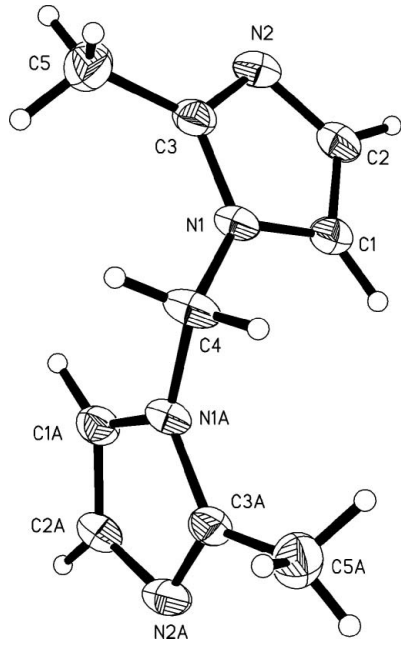

Figure 1
Drawing of the title molecule, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code (A): $1 - x, y, \frac{1}{2} - z$.]

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