

Jian Li

Department of Maths and Physics, Huangshi
Institute of Technology, Huangshi 435000,
People's Republic of ChinaCorrespondence e-mail:
hsljian2006@yahoo.com

Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.048
 wR factor = 0.123
Data-to-parameter ratio = 9.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

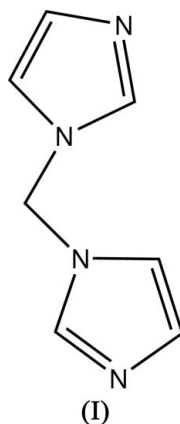
Bis(imidazol-1-yl)methane

In the title compound, $\text{C}_7\text{H}_8\text{N}_4$, the C atom of the bridging methylene group lies on a twofold rotation axis. The dihedral angle between the symmetry-related imidazole rings is $75.0(2)^\circ$. The crystal packing is stabilized by van der Waals forces.

Received 17 March 2006
Accepted 29 March 2006

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 metallic complexes have been reported, there are only a few reports on the structures of the ligands.



The title compound, (I), was prepared by using the phase-transfer organic synthesis method (Juliá *et al.*, 1984). The molecule contains two five-membered imidazole rings bridged by a methylene group (Fig. 1). Atom C4 of the bridging methylene group lies on a twofold rotation axis. The back donation of the lone pair of electrons of atom N2 may affect the C–N bond lengths and C–N–C bond angles (Table 1). The dihedral angle between the symmetry-related imidazole rings is $75.0(2)^\circ$. The crystal packing is stabilized by van der Waals forces.

Experimental

The title compound was synthesized by modifying a literature method (Diez-Barra *et al.*, 1993) and was identified by NMR. It was crystallized by slow evaporation of a chloroform–methanol (5:1 v/v) solution (yield 200 mg, 78%; m.p. 441–442 K).

Crystal data

$C_7H_8N_4$
 $M_r = 148.17$
 Orthorhombic, $P2_12_12$
 $a = 8.0357$ (18) Å
 $b = 10.545$ (2) Å
 $c = 4.3613$ (10) Å
 $V = 369.55$ (15) Å³

$Z = 2$
 $D_x = 1.332$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 293$ (2) K
 Block, colourless
 $0.49 \times 0.45 \times 0.32$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.757$, $T_{\max} = 0.998$

2176 measured reflections
 508 independent reflections
 461 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.079$
 $\theta_{\text{max}} = 27.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.123$
 $S = 1.02$
 508 reflections
 52 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0898P)^2 + 0.003P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.007$
 $\Delta\rho_{\text{max}} = 0.19$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.11 (4)

Table 1

Selected geometric parameters (Å, °).

N1—C1	1.295 (3)	N2—C3	1.375 (2)
N1—C2	1.367 (2)	N2—C4	1.444 (2)
N2—C1	1.351 (2)	C2—C3	1.342 (2)
C1—N1—C2	104.94 (16)	N1—C1—N2	112.50 (18)
C1—N2—C3	106.04 (16)	C3—C2—N1	110.81 (19)
C1—N2—C4	126.83 (14)	C2—C3—N2	105.71 (14)
C3—N2—C4	127.13 (13)	N2 ⁱ —C4—N2	112.1 (2)
C2—N1—C1—N2	-0.1 (2)	N1—C2—C3—N2	0.3 (2)
C3—N2—C1—N1	0.3 (2)	C1—N2—C3—C2	-0.3 (2)
C1—N1—C2—C3	-0.1 (2)		

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

H atoms were positioned geometrically at distances of 0.93 (CH) and 0.97 Å (CH₂) from the parent C atoms and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. Due to the absence of any significant anomalous scatterers, Friedel pairs were merged before the final refinement.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics:

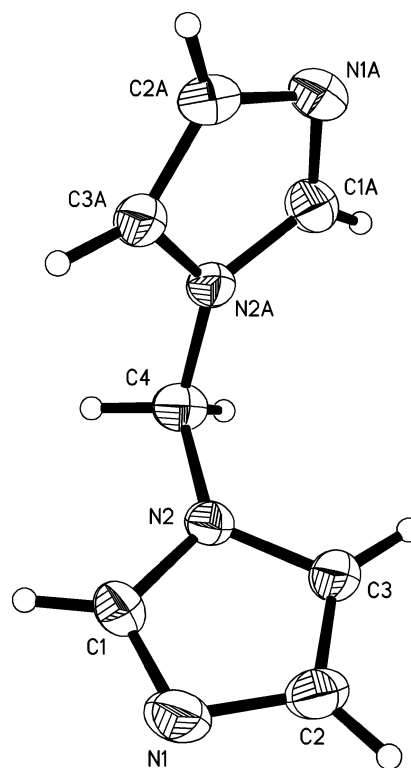


Figure 1

View of (1), with the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level [symmetry code: (A) $-x, 1 - y, z$].

SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

References

- Bruker (1998). SMART, SAINT and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
 Diez-Barra, E., Hoz, A., Sanchez-Migallon, A. & Tejada, J. (1993). *J. Chem. Soc. Perkin Trans. 1*, pp. 1079–1084.
 Effendy, M. F., Pettinari, C., Pettinari, R., Skelton, B. W. & White, A. H. (2003). *Inorg. Chem.* **42**, 112–117.
 Juliá, S., Mazo, J., Avila, I. & Elguero, J. (1984). *Org. Prep. Proc. Int.* **16**, 299–307.
 Juliá, S., Sala, P., Mazo, J. D., Sancho, M., Ochoa, C., Elguero, J., Fayet, J. & Vertut, M. (1982). *J. Heterocycl. Chem.* **19**, 1141–1145.
 Muller, M., Lork, E. & Mews, R. (2001). *Angew. Chem. Int. Ed.* **40**, 1247–1249.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
 Sorrell, T. N. & Borovik, A. S. (1987). *J. Am. Chem. Soc.* **109**, 4255–4260.