1974). Calculations performed on a FACOM M340R computer at Shionogi Research Laboratories. The final atomic coordinates and equivalent isotropic temperature factors are given in Table 1. Bond distances and angles are listed in Table 2.* A perspective view of the molecule with the atom-numbering system and a stereoscopic view of the crystal packing drawn using the program *PLUTO* (Motherwell & Clegg, 1978) are presented in Figs. 1 and 2, respectively.

**Related literature.** The absolute configuration of the title compound reported here has been referred to by Yodo, Matsushita, Ohsugi & Harada (1988).

* Lists of structure factors, anisotropic temperature factors of the non-H atoms and atomic coordinates of the H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51281 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The author thanks Dr Ohsugi for the supply of the crystals.

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# Structure of Bis[(*N*-methyl-2-imidazolyl)methyl]amine

BY JOHN F. RICHARDSON,* CHERYL A. WILSON-BLUMENBERG, KENNETH J. OBERHAUSEN, MARK S. MASHUTA AND ROBERT M. BUCHANAN*

*Department of Chemistry, University of Louisville, Louisville, Kentucky* 40292, *USA*

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**Abstract.** $C_{10}H_{15}N_5$, $M_r = 205{\cdot}26$, triclinic, $P\bar{1}$, $a = 8{\cdot}364\ (1)$, $b = 9{\cdot}148\ (1)$, $c = 7{\cdot}350\ (2)$ Å, $\alpha = 99{\cdot}92\ (2)$, $\beta = 95{\cdot}28\ (2)$, $\gamma = 94{\cdot}16\ (1)°$, $V = 549{\cdot}4\ (3)$ Å$^3$, $Z = 2$, $D_x = 1{\cdot}24$ Mg m$^{-3}$, Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å, $\mu = 0{\cdot}08$ mm$^{-1}$, $F(000) = 220$, $T = 295$ K, final $R = 0{\cdot}042$ for 1516 observed reflections. The structure of the title compound has been examined by X-ray crystallography. The compound was prepared by a nine-step synthetic procedure starting with *N*-methylimidazole and has been used to prepare biologically relevant binucleating ligands. Both *N*-methylimidazolyl moieties are planar and twisted 71·3° relative to their individual molecular least-squares planes. There are no significant intermolecular interactions and the C—C and C—N bond lengths appear to be normal.

**Experimental.** Cut arrowhead-shaped colorless crystal, 0·30 × 0·40 × 0·50 mm, Enraf–Nonius CAD-4 diffractometer, graphite monochromator, Mo $K\alpha$ radiation, unit-cell parameters from least-squares refinement of 25 reflections with $12 < \theta < 19{\cdot}5°$, space group $P\bar{1}$ determined from intensity data and successful solution and refinement of the structure; 2200 data collected, 1915 unique reflections, 1516 observed at the $3\sigma(I)$ level [$\sigma(I)$ from counting statistics]; $\theta_{max} = 25°$, scan range $(0{\cdot}8 + 0{\cdot}344\tan\theta)°$, $\omega/2\theta$ scans, variable scan speed 1–3° min$^{-1}$; three standard reflections measured every 3600 s of X-ray exposure time, variation −6·7%, linear decay correction applied; data collected $\pm h$, $\pm k$, $-l$ to max. indices of 9, 10, 8. Data corrected for background and Lp; empirical absorption correction based on a series of $\psi$ scans, relative transmission coefficients ranging from 0·977 to 1·000 with average value of 0·987; secondary-extinction correction applied (Zachariasen, 1963), final coefficient refined in least squares was $8{\cdot}8\ (4) \times 10^{-6}$; intensities of equivalent reflections averaged, agreement factors for averaging of 275 observed and accepted reflections was 0·6% based on *I*. Structure solved by direct methods, all non-H located from *E* map, model refined by full-matrix least squares based on *F*, minimizing the function $\sum w(|F_o| - |F_c|)^2$; $w$ defined as $[\sigma^2(F_o) + (0{\cdot}15F_o)^2 + 3{\cdot}0]^{-1}$, *SDP*/VAX package of programs

* To whom correspondence should be addressed.

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Table 1. *Positional and isotropic thermal parameters for non-*H *atoms*

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$$\tfrac{4}{3}[a^2B(1,1) + \cdots ab(\cos\gamma)B(1,2) + \cdots].$$

| | $x$ | $y$ | $z$ | $B_{eq}$(Å$^2$) |
|---|---|---|---|---|
| N1 | 0·0847 (2) | 0·1953 (2) | 0·3240 (2) | 3·89 (3) |
| N2 | 0·2339 (2) | −0·0184 (2) | 0·6105 (2) | 4·55 (3) |
| N3 | 0·4061 (2) | 0·1665 (2) | 0·5784 (2) | 4·13 (3) |
| N4 | −0·2407 (2) | 0·3168 (2) | 0·0959 (2) | 5·42 (4) |
| N5 | −0·0438 (2) | 0·4861 (2) | 0·2279 (2) | 4·16 (3) |
| C1 | 0·1931 (2) | 0·0763 (2) | 0·3132 (3) | 4·57 (4) |
| C2 | 0·2764 (2) | 0·0724 (2) | 0·4994 (2) | 3·67 (3) |
| C3 | 0·3412 (2) | 0·0210 (2) | 0·7685 (3) | 5·05 (4) |
| C4 | 0·4470 (2) | 0·1333 (2) | 0·7499 (3) | 4·80 (4) |
| C5 | 0·4864 (3) | 0·2820 (2) | 0·4955 (4) | 6·22 (5) |
| C6 | 0·0305 (3) | 0·2246 (2) | 0·1400 (3) | 4·75 (4) |
| C7 | −0·0859 (2) | 0·3408 (2) | 0·1529 (2) | 4·12 (4) |
| C8 | −0·2994 (3) | 0·4535 (3) | 0·1380 (3) | 5·89 (5) |
| C9 | −0·1811 (3) | 0·5590 (2) | 0·2191 (3) | 5·21 (4) |
| C10 | 0·1156 (2) | 0·5552 (2) | 0·3075 (3) | 5·20 (5) |

Table 2. *Bond distances* (Å) *and angles* (°)

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N1 | C1 | | 1·464 (2) | N4 | C8 | | 1·374 (3) |
| N1 | C6 | | 1·462 (2) | N5 | C7 | | 1·356 (2) |
| N2 | C2 | | 1·314 (3) | N5 | C9 | | 1·371 (3) |
| N2 | C3 | | 1·379 (2) | N5 | C10 | | 1·458 (2) |
| N3 | C2 | | 1·354 (2) | C1 | C2 | | 1·485 (3) |
| N3 | C4 | | 1·366 (3) | C3 | C4 | | 1·340 (3) |
| N3 | C5 | | 1·461 (3) | C6 | C7 | | 1·490 (3) |
| N4 | C7 | | 1·314 (2) | C8 | C9 | | 1·350 (3) |
| C1 | N1 | C6 | 111·7 (1) | N2 | C2 | C1 | 125·5 (1) |
| C2 | N2 | C3 | 105·4 (1) | N3 | C2 | C1 | 123·4 (2) |
| C2 | N3 | C4 | 107·1 (2) | N2 | C3 | C4 | 110·1 (2) |
| C2 | N3 | C5 | 126·2 (2) | N3 | C4 | C3 | 106·4 (2) |
| C4 | N3 | C5 | 126·7 (1) | N1 | C6 | C7 | 110·9 (1) |
| C7 | N4 | C8 | 104·9 (2) | N4 | C7 | N5 | 111·4 (2) |
| C7 | N5 | C9 | 107·4 (1) | N4 | C7 | C6 | 125·1 (2) |
| C7 | N5 | C10 | 127·6 (2) | N5 | C7 | C6 | 123·4 (2) |
| C9 | N5 | C10 | 125·1 (2) | N4 | C8 | C9 | 111·2 (2) |
| N1 | C1 | C2 | 110·7 (1) | N5 | C9 | C8 | 105·3 (2) |
| N2 | C2 | N3 | 111·0 (2) | | | | |

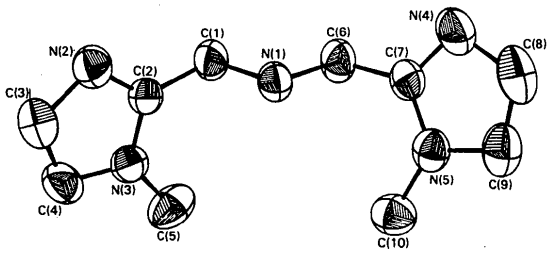


Fig. 1. Numbering scheme and *ORTEP* (Johnson, 1965) drawing (50% thermal ellipsoids) of the title compound.

(Frenz, 1978) using VAX 11/750; H atoms included in positions located from difference Fourier map and added to the structure factor calculations with isotropic thermal parameters fixed at $1·3 \times B_{eq}$ of the bonded atom; disordered $CH_3$ groups each with 70:30 occupancy of H atoms; H-atom parameters not refined; all non-H atoms refined using anisotropic thermal parameters, model converged using 1516 reflections and 137 variable parameters, $R = 0·042$, $wR = 0·054$, max. $(\Delta/\sigma) < 0·01$, $S = 1·76$, max. residual electron density 0·18 e Å$^{-3}$ with an estimated error based on $F$ (Cruickshank, 1949) of 0·03. Scattering factors were those of Cromer & Waber (1974). Anomalous-dispersion corrections were included in $F_c$ (Ibers & Hamilton; 1964), using values of $f'$ and $f''$ from Cromer (1974). Atomic parameters for non-H atoms may be found in Table 1 while bond lengths and angles for the non-H atoms are listed in Table 2.* Fig. 1 shows the numbering scheme and *ORTEP* (Johnson, 1965) drawing of the molecule.

**Related literature.** A preliminary account of the use of the title compound to prepare binucleating ligands has been published (Buchanan, Oberhausen & Richardson, 1988). This is the first structure reported on a free tridentate-$N_3$ imidazolyl ligand. Copper(I) complexes of similar ligands have been reported (Dadigan, McKee & Reed, 1982; Sorrell & Jameson, 1982).

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond lengths and distances for H atoms, and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51192 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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