N,N′-Dimethylpiperazine, grown at 270 K and studied at 220 K

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Key indicators

Single-crystal X-ray study
$T = 220$ K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.107
Data-to-parameter ratio = 16.6

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

The crystal structure of the title compound, $MeNC_4H_8NMe$ or $C_6H_{14}N_2$, which is liquid under ambient conditions, has been determined at low temperature. The molecule occupies a special position on a crystallographic inversion centre. The piperazine ring has an almost ideal chair conformation, with the absolute values of the endocyclic torsion angles in the range 57.4–58.6°. No close C—H···N contacts are observed in the crystal structure.

## Comment

N,N′-Dimethylpiperazine has been observed in 36 crystal structures in the April 2002 Release (Version 5.23) of the Cambridge Structural Database (Allen & Kennard, 1993), although the structure of the pure compound has not previously been determined. Of these database structures, 24 are observed to exist in the diammonium cationic form [e.g. CSD refcodes GOPSEJ, GOPSOT, GOPSUZ and GOPTEK (Troyanov et al., 1999)], and six have both amino groups ligated to a metal [e.g. CUCSAU (Clegg et al., 2000) and MPIPDC (Hassel & Pedersen, 1959)]. Three additional structures have one amino N atom protonated and the second ligated to a metal cation [QEFXOO (Clemente et al., 1999), QISFED and QISFON (Marzotto et al., 2001)]. This leaves three structures [DOSKAX (Gall et al., 1985) and GERWEF and GERWIJ (Yabuki et al., 1988)] with the compound in its neutral form, of which two are cocrystals of different enantiomers (GERWEF and GERWIJ). In all three structures, the amino groups are involved as hydrogen-bond acceptors.

(I)
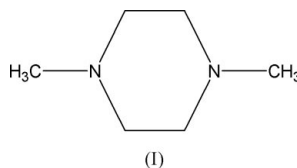
The molecule of N,N′-dimethylpiperazine, (I), as determined by the present study (Fig. 1), occupies a special position in a crystallographic inversion centre. The piperazine ring has an almost ideal chair conformation with the endocyclic torsion angles showing alternating signs and absolute values within the narrow interval of 57.4–58.6°.

In pure N,N′-dimethylpiperazine, no hydrogen-bond donors exist. Nevertheless, it might be expected that close C—H···N contacts would be observed from the methyl groups. This proves not to be the case, with no contacts of less than the sum of the van der Waals radii of the closest atoms observed in this structure. The shortest non-bonded contact to the amino N
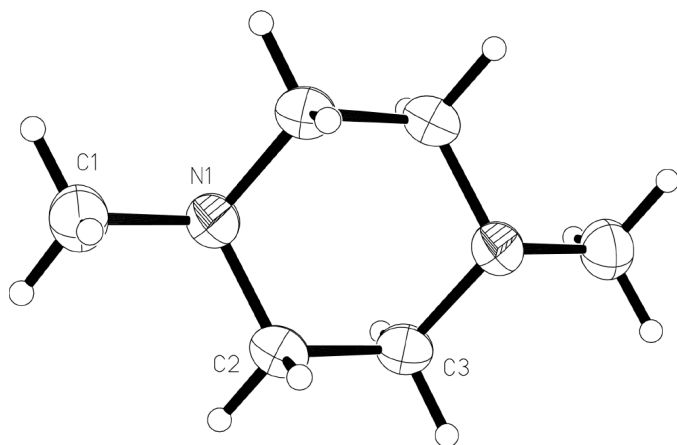
Figure 1
A view of N,N′-dimethylpiperazine. Displacement ellipsoids are drawn at the 30% probability level. The unlabelled atoms are related by an inversion centre in the centre of the molecule.

atom is $N1 \cdots H1A^i—C1^i$ [symmetry code (i): $x, \frac{1}{2} - y, \frac{1}{2} + z$] is 2.88 Å to the geometrically placed H atom and 3.6646 (17) Å to the C atom. The crystal packing process can, therefore, be said to be governed by weak van der Waals interactions. This is entirely consistent with the previously reported crystal structure of trimethylamine, determined by Blake *et al.* (1984) and redetermined by Boese *et al.* (1998), where voids are observed in the crystal structure in the expected position of the N-atom lone-pair. The lower than expected density of 1.053 Mg m^{-3} of (I) is comparable with that of 0.858 Mg m^{-3} of trimethylamine, observed by Blake *et al.* (1984).

Experimental

N,N′-Dimethylpiperazine was used as received from Aldrich without any further purification. An X-ray quality crystal was grown *in situ* at 270 K from a small seed obtained by melting back the sample of the frozen liquid in a thin capillary of 0.30 mm diameter.

Crystal data

$C_6H_{14}N_2$	$D_x = 1.053$ Mg m^{-3}
$M_r = 114.19$	Cu $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 85
$a = 5.8083$ (9) Å	reflections
$b = 10.9298$ (19) Å	$\theta = 15.0$–$22.0°$
$c = 5.7575$ (8) Å	$\mu = 0.50$ mm^{-1}
$\beta = 99.903$ (12)°	$T = 220$ (2) K
$V = 360.06$ (10) Å^3	Cylinder, colourless
$Z = 2$	0.15 mm (radius)

Data collection

Stoe Stadi-4 four-circle diffractometer	590 reflections with $I > 2\sigma(I)$
ω–2θ scans	$R_{int} = 0.027$
Absorption correction: multi-scan [*MULABS* (Spek, 1998), based on the method of Blessing (1995)]	$\theta_{max} = 69.7°$
	$h = -7 \rightarrow 7$
	$k = -13 \rightarrow 13$
	$l = -6 \rightarrow 6$
$T_{min} = 0.761$, $T_{max} = 0.840$	3 standard reflections
2463 measured reflections	frequency: 30 min
646 independent reflections	intensity decay: 6%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.053P)^2 + 0.0372P]$
$R[F^2 > 2\sigma(F^2)] = 0.038$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.107$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.10$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
646 reflections	$\Delta\rho_{min} = -0.10$ e Å^{-3}
39 parameters	Extinction correction: *SHELXL*97
H-atom parameters constrained	Extinction coefficient: 0.087 (9)

H atoms were located in difference Fourier maps, then positioned geometrically and allowed to ride on their respective parent atoms.

Data collection: *DIF*4 (Stoe & Cie, 1990); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1990); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*.

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