

133.1 (1)°, are smaller than those in similar structures found in the Cambridge Structural Database (Clarke, Jewers & Jones 1980; Codding, Szkaradzinska & Roszak 1988; Fukamiya, Okano & Aratani 1986).

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Structure of *N,N'*-Bis(2-hydroxyethyl)piperazine

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Abstract. 1,4-Piperazinediethanol, C₁₈H₁₈N₂O₂, *M_r* = 174.24, orthorhombic, *Pbca*, *a* = 9.328 (1), *b* = 12.106 (2), *c* = 8.253 (1) Å, *V* = 931.9 (4) Å³, *Z* = 4, *D_m* = 1.236, *D_x* = 1.239 g cm⁻³, λ(Cu Kα) = 1.5418 Å, μ = 7.32 cm⁻¹, *F*(000) = 384, *T* = 293 K, final *R* = 0.052 for 911 independent reflections. The molecule is centrosymmetric with the piperazine ring in a chair form. In the ring the mean N—C length is 1.471 Å and the C—N—C angle is 108.2°. The hydroxyethyl groups are in equatorial positions.

Experimental. Colorless prisms from an ethyl acetate solution. Crystal 0.4 × 0.35 × 0.6 mm (m.p. 408.3–409.1 K). *D_m* measured by flotation. Rigaku AFC-5 four-circle diffractometer, graphite-monochromated Cu Kα radiation. Intensity data collected in ω-2θ scan mode (2θ_{max} = 120°). Unit-cell dimensions by least-squares procedure based on 2θ values (29 < 2θ < 56°) of 48 reflections. Total of 95 reflections measured of which 911 independent (0 ≤ *h* ≤ 10, -13 ≤ *k* ≤ 0, 0 ≤ *l* ≤ 9). No systematic fluctuation in

333, 400 and 004 standard reflections, monitored every 200 reflections. No absorption correction.

Structure determined using *SHELXS86* (Sheldrick, 1986). Block-diagonal and full-matrix least-squares refinement (*HBL5-V*; Ashida, 1979). Σ*w*(*F_o* - *k*|*F_c*)² minimized. Weighting scheme: *w* = 0.0 for *F_o* = 0.0, *w* = 1 for |*F_o*| < 10.0, *w* = (10.0/|*F_o*|)² for |*F_o*| > 10.0. Subsequent difference Fourier maps revealed positions for all H atoms. Non-H atoms refined with anisotropic temperature factors, and H atoms with isotropic ones. Final *R* = 0.052, *wR* = 0.065, *S* = 0.25, using 704 observations with |*F_o*| ≥

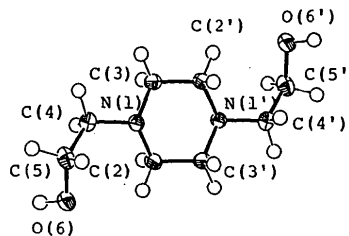


Fig. 1. Numbering scheme and the thermal ellipsoids. Thermal vibration ellipsoids are set to 50% probability (Johnson, 1965).

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Table 1. Atomic coordinates and equivalent isotropic thermal parameters (\AA^2) of the non-H atoms with e.s.d.'s in parentheses
$$B_{\text{eq}} = \frac{1}{3} \sum_i \sum_j \beta_{ij} \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	B_{eq}
N(1)	0.54041 (15)	0.38421 (12)	0.0047 (2)	1.97 (3)
C(2)	0.4251 (2)	0.42902 (15)	0.1069 (2)	2.37 (4)
C(3)	0.6452 (2)	0.47274 (15)	0.0251 (2)	2.42 (4)
C(4)	0.6125 (2)	0.28927 (16)	0.0806 (2)	2.64 (4)
C(5)	0.5229 (2)	0.18449 (16)	0.0871 (2)	2.91 (5)
O(6)	0.41560 (14)	0.18422 (11)	0.2090 (2)	2.95 (4)

Table 2. Intramolecular interatomic distances (\AA) and angles ($^\circ$) with e.s.d.'s in parentheses

N(1)—C(2)	1.471 (2)	N(1)—C(3)	1.471 (2)
N(1)—C(4)	1.471 (2)	C(4)—C(5)	1.520 (3)
C(5)—O(6)	1.419 (3)	C(2)—C(3')	1.514 (2)
C(2)—N(1)—C(3)	108.2 (1)	C(2)—N(1)—C(4)	112.2 (1)
C(3)—N(1)—C(4)	109.7 (1)	N(1)—C(4)—C(5)	114.6 (2)
C(4)—C(5)—O(6)	114.5 (2)	N(1)—C(2)—C(3')	110.5 (2)
N(1)—C(3)—C(2)	111.0 (2)		

$3\sigma(F_o)$ and 91 variables. $(\Delta/\sigma)_{\text{max}} = 0.03$. Final difference map contained no peak higher than 0.3 e \AA^{-3} . Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). All the calculations were performed on an NEC ACOS-930 computer of the Protein Engineering Research Center, Institute for Protein Research, Osaka University.

The numbering scheme and the thermal ellipsoids of all the atoms are illustrated in Fig. 1. Positional parameters are given in Table 1.* Bond lengths and angles are given in Table 2.

* Lists of structure amplitudes, anisotropic thermal parameters for non-H atoms, and positional parameters and isotropic thermal parameters for all H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55003 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Related literature. Gas electron-diffraction studies: Davis & Hassel (1963); Yokozeki & Kuchitsu (1971). IR spectra studies: Cook, Jones, Katritzky, Manas, Richards, Sparrow & Trepanier (1973); Imbach, Jones, Katritzky & Wyatt (1967); Baldock & Katritzky (1968); Bishop, Sutton, Dineen, Jones, Katritzky & Wyatt (1967). Related compounds: Okamoto, Sekido, Itoh, Noguchi & Hirokawa (1979); Okamoto, Sekido, Ono, Noguchi & Hirokawa (1982); Sekido, Okamoto & Hirokawa (1985).

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Structure of Concanamycin A Pentahydrate

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Abstract. Concanamycin A was obtained from the culture broth of *Streptomyces diastatochromogenese* PA-48098. Three crystal forms of concanamycin A

were obtained, (Ia) from methanol–water, (II) from ethanol–water and (I) on drying (Ia). (I): $\text{C}_{46}\text{H}_{75}\text{NO}_{14} \cdot 5\text{H}_2\text{O}$, $M_r = 956.17$, monoclinic, $P2_1$, a