

The atomic parameters are given in Table 1.* The bond lengths and angles are listed in Table 2. Fig. 1 is a stereoscopic view of the molecule, showing the numbering of the atoms (*PLUTO*, Motherwell & Clegg, 1978).

Related literature. There are only eight structures which contain the bicyclo[4.2.0]octan-7-one skeleton (Cambridge Structural Database, version 4.10: Allen *et al.*, 1979). From these, 8-[(2,2-dimethyl-3-oxocyclohexyl)hydroxymethyl]-1-methylbicyclo[4.2.0]octan-7-one (Fair, Clark & Nikaido, 1985) is the only structure with monosubstitution at C8; in this

molecule the puckering of the cyclobutanone ring is 26.1 (2)°.

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* Lists of structure factors, anisotropic thermal parameters, bond lengths and angles, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52873 (21 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1990). C46, 1946–1947

Structure of 2,3-Dimethylquinoxaline

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(Received 12 February 1990; accepted 2 April 1990)

Abstract. C₁₀H₁₀N₂, *M_r* = 158.20, monoclinic, *C*2/*c*, *a* = 7.641 (2), *b* = 9.896 (1), *c* = 11.480 (1) Å, β = 99.10 (1)°, *V* = 857.12 (25) Å³, *Z* = 4, *D_x* = 1.226 g cm⁻³, λ(Mo *K*α) = 0.71069 Å, μ = 0.699 cm⁻¹, *F*(000) = 336, *T* = 291 K, *R* = 0.0396 for 623 unique observed reflections. The structure consists of 2,3-dimethylquinoxaline molecules oriented about the twofold axes. The molecule is planar.

Experimental. Crystals of 2,3-dimethylquinoxaline (hereafter abbreviated DMQ) were crystallized from acetonitrile. An Enraf–Nonius CAD-4 diffractometer was used with graphite-monochromatized Mo *K*α radiation. The crystal size was 0.20 × 0.30 × 0.35 mm. Unit-cell parameters were obtained by least-squares fit of the setting angles of 25 reflections in the θ range 3 < 2θ < 13°. The intensities of 4105 reflections were measured (sin θ ≤ 30°, -9 ≤ *h* ≤ 9, 0 ≤ *k* ≤ 11, 0 ≤ *l* < 13, ω-2θ scan mode). No significant variation (< 3%) was found in the intensities of the intensity control reflections 312, 222 and 110.

The data were corrected for Lorentz and polarization effects but no absorption correction was applied. 1654 reflections with |*F*| ≥ 3σ(*F*) were used in the calculations, *R*_{int} = 0.040. The structure was solved with multiresolution direct methods (Sheldrick, 1986), and refined using full-matrix least-squares methods (Sheldrick, 1976), minimizing Σ*w*(|*F_o*| - |*F_c*|)², *w* = 6.8151/[σ²(*F*) + 0.00007*F*²]. Heavy atoms were refined with anisotropic and H atoms with isotropic temperature factors; 76 parameters were varied. The refinement converged to *R* = 0.0396, *wR* = 0.0402, (Δ/σ)_{max} = 0.002, (Δ/σ)_{mean} = 0.001 and (Δρ)_{max}/(Δρ)_{min} = +0.12/-0.12 e Å⁻³. Fractional coordinates and equivalent isotropic temperature coefficients for non-H atoms are given in Table 1.* The

* Lists of atomic parameters for H atoms, anisotropic thermal parameters for non-H atoms and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52920 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Fractional coordinates ($\times 10^4$) and equivalent temperature coefficients ($\times 10^4$) for non-H atoms

	x	y	z	$U_{eq}(\text{\AA}^2)$
N1	956 (2)	6209 (1)	3651 (1)	631 (5)
C2	481 (2)	7396 (2)	3076 (1)	577 (5)
C3	487 (2)	5080 (2)	3092 (1)	607 (5)
C4	946 (2)	8634 (2)	3641 (2)	715 (8)
C5	474 (2)	9804 (3)	3076 (2)	833 (8)
C6	994 (3)	3786 (2)	3723 (2)	828 (9)

Table 2. Bond lengths (\AA) and angles ($^\circ$)

C2—N1	1.368 (2)	N1—C2—C2*	120.8 (2)
C3—N1	1.310 (2)	N1—C2—C4	119.8 (1)
C2—C2*	1.408 (2)	C2—N1—C3	117.7 (1)
C4—C2	1.405 (3)	N1—C3—C3*	121.5 (2)
C3—C3*	1.443 (2)	N1—C3—C6	117.7 (1)
C6—C3	1.492 (3)	C2*—C2—C4	119.3 (2)
C5—C4	1.348 (3)	C2—C4—C5	119.9 (2)
C5—C5'	1.404 (3)	C3*—C3—C6	120.9 (2)
C6—C6*	2.974 (3)	C4—C5—C5*	120.8 (2)

*Atom generated by symmetry operation: $-x, y, \frac{1}{2}-z$.

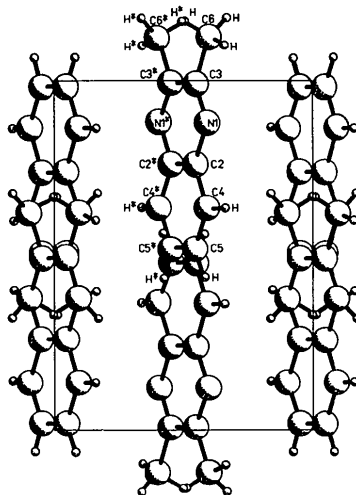


Fig. 1. A projection of the unit-cell content on the ab plane with the labelling of the atoms.

molecular geometry is given in Table 2 with atom labelling in Fig. 1. The packing of the molecules in the unit cell is also given in Fig. 1. The figure was drawn with *PLUTO* (Motherwell, 1972).

Related literature. Crystal structures containing 2,3-disubstituted derivatives of quinoxaline have aroused

considerable interest because of the repulsion between the neighbouring substituents (Visser, Vos, de Grooth & Wynberg, 1968; Visser & Vos, 1971; Lipkowski, Herbich & Andreetti, 1985; Krigier, Kocak & Bekaroglu, 1985). The C6—C6* distance (Fig. 1) is 2.974 (3) \AA . It is shorter than in the other 2,3-disubstituted derivatives of quinoxaline, but the repulsion between the two methyl groups still causes significant deformations of the valence angles about C6 and C6*.

We thank the British Council for a grant to KW.

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Acta Cryst. (1990). **C46**, 1947–1949

Die Struktur eines α -thiolierten SAMP-Hydrazons

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(Eingegangen am 18. Juli 1989; angenommen am 5. April 1990)

Abstract. (2*S*)-(+) -2-Methoxymethyl-1-[(2*R*)-2-methylthio-1-phenyl-1-propylideneamino]pyrroli-

dine, $C_{16}H_{24}N_2OS$, $M_r = 292.4$, orthorhombic, $P2_12_12_1$, $a = 6.307(2)$, $b = 11.243(1)$, $c = 23.592(8)$ \AA , $V = 1672.91$ \AA^3 , $Z = 4$, $D_x = 1.161$ g cm^{-3} , $\lambda(\text{Mo K}\alpha) = 0.71069$ \AA , $\mu = 1.54$ cm^{-1} , $F(000) =$

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0108-2701/90/101947-03\$03.00

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