Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

3-Methyl-1-(prop-2-en-1-yl)quinoxalin-2(1*H*)-one

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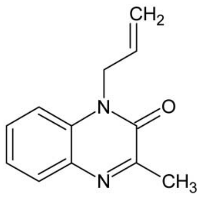
Received 11 June 2010; accepted 18 June 2010

Key indicators: single-crystal X-ray study; T = 296 K; P = 0.0 kPa; mean σ(C–C) = 0.002 Å; R factor = 0.051; wR factor = 0.151; data-to-parameter ratio = 18.5.

In the molecule of the title compound, $C_{12}H_{12}N_2O$, the quinoxaline ring is planar with an r.m.s. deviation of 0.007 (15) Å. The dihedral angle between the quinoxaline and propenyl planes is 82.1 (2)°. The crystal packing is stabilized by offset π–π stacking between the quinoxaline rings [centroid–centroid distance = 3.8832 (9) Å].

Related literature

For biological activity of quinoxaline derivatives, see: Kleim *et al.* (1995). For their antitumor, and antituberculous properties, see: Abasolo *et al.* (1987); Rodrigo *et al.* (2002). For the antifungal, herbicidal, antidyslipidemic and anti-oxidative activities of quinoxaline derivatives, see: Jampilek *et al.* (2005); Sashidhara *et al.* (2009); Watkins *et al.* (2009). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{12}H_{12}N_2O$
M_r = 200.24
Monoclinic, $P2_1/c$
a = 5.0722 (5) Å
b = 13.4707 (13) Å
c = 15.0507 (13) Å
β = 95.082 (5)°
V = 1024.31 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.32 × 0.31 × 0.13 mm

Data collection

Bruker X8 APEXII CCD area-detector diffractometer
11850 measured reflections
2546 independent reflections
1726 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.151
S = 1.08
2546 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.23 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.17 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *publCIF* (Westrip, 2010).

The authors thank the CNRST of Morocco for making this work possible.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2579).

References

Abasolo, M. I., Gaozza, C. H. & Fernandez, B. M. J. (1987). *Heterocycl. Chem.* **24**, 1771–1775.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Jampilek, J., Dolezal, M., Kunes, J., Buchta, V. & Kralova, K. (2005). *Med. Chem.* **1**, 591–599.
Kleim, J. P., Bender, R., Kirsch, R., Meichsner, C., Paessens, A., Rosner, M., Rubsamen Waigmann, H., Kaiser, R., Wichers, M., Schneweis, K. E., Winkler, I. & Riess, G. (1995). *Antimicrob. Agents Chemother.* **39**, 2253–2257.
Rodrigo, G. A., Robinshon, A. E., Hedrera, M. E., Kogan, M., Sicardi, S. M. & Fernaandez, B. M. (2002). *Trends Heterocycl. Chem.* **8**, 137–143.
Sashidhara, K. V., Kumar, A., Bhatia, G., Khan, M. M., Khanna, A. K. & Saxena, J. K. (2009). *Eur. J. Med. Chem.* **44**, 1813–1818.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Watkins, A. J., Nicol, G. W. & Shawa, L. J. (2009). *Soil Biol. Biochem.* **41**, 580–585.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**. Submitted.

doi:10.1107/S1600536810023640

supplementary materials

Acta Cryst. (2010). E**66**, o1767 [**doi:10.1107/S1600536810023640**]

3-Methyl-1-(prop-2-en-1-yl)quinoxalin-2(1*H*)-one

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Comment

Quinoxaline derivatives are a very important class of nitrogen-containing compounds and have been widely used in dyes, pharmaceuticals and electrical/photochemical materials. Quinoxaline ring moiety constitute part of the chemical structures of various antibiotics such as Echinomycin, Levomycin and Actinoleutin that are known to inhibit growth of gram positive bacteria and are active against various transplantable tumors.

Quinoxaline derivatives were found to exhibit antimicrobial [Kleim *et al.* 1995], antitumor [Abasolo *et al.* 1987], and antituberculous activity [Rodrigo *et al.*2002]. They, also, exhibit interesting antifungal, herbicidal, Antidyslipidemic and antioxidative activities of quinoxaline derivatives, see: (Jampilek *et al.* 2005, Sashidhara *et al.* 2009, Watkins *et al.* 2009).

The dihedral angle between the quinoxaline and propenyl planes is 82.1 (2) (Fig. 1). Bond lengths and angles in title molecule are normal (Allen *et al.*, 1987). The crystal packing is stabilized by offset π-π stacking between the quinoxalin rings.

Experimental

To a solution of 3-methylquinoxali-2(1*H*)-one (1 g) in 20 ml of dimethylformamide was added allylchloride (0.85 ml),K2CO3 (0.95 g) and catalytic amont of tetrabutylammonium bromide.The mixture was stirred at room temperature for 24 h.Then the solvent was remdove under reduce pressure,the residue was cristallized in ethanol to afford the product.

Refinement

Although found in a difference map, H atoms were introduced in calculated positions and treated as riding with C—H = 0.96 Å for methyl groups, C—H = 0.93 Å for aromatic and C—H = 0.97 Å for methine with U iso (H) = $1.2U_{eq}$ (aromatic, methine) or U iso (H) = $1.5U_{eq}$ (methyl).

Figures

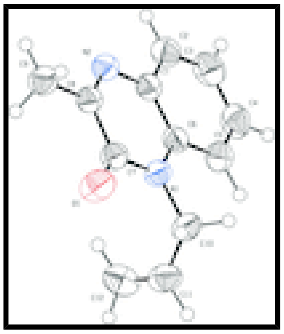

Fig. 1. : Molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

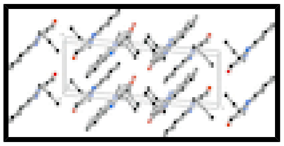

Fig. 2. : Packing view of the crystal structure of the title compound.

3-Methyl-1-(prop-2-en-1-yl)quinoxalin-2(1*H*)-one

Crystal data

$C_{12}H_{12}N_2O$

$M_r = 200.24$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 5.0722\ (5)$ Å

$b = 13.4707\ (13)$ Å

$c = 15.0507\ (13)$ Å

$\beta = 95.082\ (5)°$

$V = 1024.31\ (17)$ Å^3

$Z = 4$

$F(000) = 424$

$D_x = 1.298$ Mg m^{-3}

Melting point: 1486 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2764 reflections

$\theta = 2.4–27.4°$

$\mu = 0.09$ mm^{-1}

$T = 296$ K

Block, colourless

0.32 × 0.31 × 0.13 mm

Data collection

Bruker X8 APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

graphite

φ and ω scans

11850 measured reflections

2546 independent reflections

1726 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.049$

$\theta_{\text{max}} = 28.3°$, $\theta_{\text{min}} = 2.7°$

$h = -6 \rightarrow 6$

$k = 0 \rightarrow 17$

$l = 0 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.151$

$S = 1.08$

2546 reflections

137 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0723P)^2 + 0.0888P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.23$ e Å^{-3}

$\Delta\rho_{\text{min}} = -0.17$ e Å^{-3}

Special details

Experimental. The data collection nominally covered a sphere of reciprocal space, by a combination of seven sets of exposures; each set had a different φ angle for the crystal and each exposure covered 0.5° in ω and 30 s in time. The crystal-to-detector distance was 37.5 mm.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimatedusing the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL datawill be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.3390 (2)	0.34712 (9)	0.06022 (9)	0.0657 (4)
N1	−0.0193 (2)	0.29591 (9)	0.16502 (8)	0.0408 (3)
N2	0.1311 (2)	0.49458 (9)	0.18738 (8)	0.0445 (3)
C1	0.2649 (3)	0.41959 (11)	0.23590 (9)	0.0408 (3)
C2	0.4769 (3)	0.44552 (13)	0.29645 (10)	0.0514 (4)
H2	0.5253	0.5119	0.3030	0.062*
C3	0.6150 (3)	0.37488 (15)	0.34638 (11)	0.0589 (5)
H3	0.7560	0.3931	0.3868	0.071*
C4	0.5434 (3)	0.27599 (15)	0.33625 (11)	0.0579 (5)
H4	0.6364	0.2278	0.3704	0.069*
C5	0.3375 (3)	0.24845 (13)	0.27651 (11)	0.0503 (4)
H5	0.2932	0.1817	0.2698	0.060*
C6	0.1937 (3)	0.31975 (11)	0.22568 (9)	0.0395 (3)
C7	−0.1541 (3)	0.36731 (11)	0.11482 (10)	0.0441 (4)
C8	−0.0643 (3)	0.47053 (11)	0.13088 (9)	0.0424 (4)
C9	−0.2158 (3)	0.54800 (12)	0.07845 (11)	0.0543 (4)
H9A	−0.3878	0.5548	0.0997	0.081*
H9B	−0.2343	0.5293	0.0167	0.081*
H9C	−0.1233	0.6101	0.0850	0.081*
C10	−0.1160 (3)	0.19385 (11)	0.15522 (11)	0.0483 (4)
H10A	−0.3032	0.1956	0.1355	0.058*
H10B	−0.0975	0.1621	0.2133	0.058*
C11	0.0207 (3)	0.13211 (13)	0.09201 (12)	0.0578 (5)
H11	−0.0243	0.0652	0.0896	0.069*
C12	0.1942 (4)	0.16040 (15)	0.04015 (13)	0.0669 (5)
H12A	0.2467	0.2265	0.0398	0.080*
H12B	0.2672	0.1147	0.0030	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0682 (8)	0.0524 (8)	0.0700 (8)	−0.0060 (6)	−0.0296 (7)	0.0027 (6)
N1	0.0443 (6)	0.0358 (7)	0.0413 (6)	−0.0016 (5)	−0.0024 (5)	0.0006 (5)
N2	0.0518 (7)	0.0402 (7)	0.0407 (6)	−0.0005 (5)	−0.0013 (5)	−0.0018 (5)
C1	0.0435 (7)	0.0433 (9)	0.0353 (7)	0.0004 (6)	0.0020 (6)	−0.0008 (6)
C2	0.0527 (9)	0.0550 (10)	0.0452 (8)	−0.0061 (7)	−0.0038 (7)	−0.0033 (7)
C3	0.0527 (9)	0.0755 (13)	0.0458 (9)	−0.0016 (8)	−0.0107 (7)	−0.0006 (8)
C4	0.0592 (10)	0.0648 (12)	0.0474 (9)	0.0098 (8)	−0.0080 (7)	0.0103 (8)
C5	0.0568 (9)	0.0471 (9)	0.0460 (8)	0.0046 (7)	−0.0014 (7)	0.0053 (7)
C6	0.0416 (7)	0.0415 (9)	0.0352 (7)	0.0006 (6)	0.0026 (6)	−0.0005 (6)
C7	0.0464 (8)	0.0423 (9)	0.0420 (8)	0.0003 (6)	−0.0045 (6)	−0.0002 (6)
C8	0.0487 (8)	0.0398 (8)	0.0380 (7)	0.0027 (6)	0.0003 (6)	−0.0005 (6)
C9	0.0653 (10)	0.0439 (9)	0.0518 (9)	0.0069 (7)	−0.0059 (8)	0.0015 (7)
C10	0.0488 (8)	0.0387 (9)	0.0560 (9)	−0.0052 (6)	−0.0032 (7)	0.0022 (7)
C11	0.0625 (10)	0.0455 (10)	0.0633 (10)	−0.0042 (8)	−0.0060 (9)	−0.0077 (8)
C12	0.0696 (11)	0.0701 (13)	0.0602 (11)	−0.0030 (9)	0.0008 (9)	−0.0162 (9)

Geometric parameters (Å, °)

O1—C7	1.2215 (18)	C5—C6	1.393 (2)
N1—C7	1.3683 (19)	C5—H5	0.9300
N1—C6	1.3889 (18)	C7—C8	1.476 (2)
N1—C10	1.4629 (19)	C8—C9	1.482 (2)
N2—C8	1.2887 (18)	C9—H9A	0.9600
N2—C1	1.3881 (19)	C9—H9B	0.9600
C1—C2	1.391 (2)	C9—H9C	0.9600
C1—C6	1.397 (2)	C10—C11	1.481 (2)
C2—C3	1.367 (2)	C10—H10A	0.9700
C2—H2	0.9300	C10—H10B	0.9700
C3—C4	1.386 (3)	C11—C12	1.285 (3)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.368 (2)	C12—H12A	0.9300
C4—H4	0.9300	C12—H12B	0.9300
C7—N1—C6	121.48 (13)	O1—C7—C8	121.81 (14)
C7—N1—C10	117.26 (12)	N1—C7—C8	116.08 (13)
C6—N1—C10	121.20 (12)	N2—C8—C7	123.57 (13)
C8—N2—C1	118.41 (13)	N2—C8—C9	120.44 (14)
N2—C1—C2	118.39 (14)	C7—C8—C9	115.99 (13)
N2—C1—C6	122.20 (13)	C8—C9—H9A	109.5
C2—C1—C6	119.41 (14)	C8—C9—H9B	109.5
C3—C2—C1	120.95 (16)	H9A—C9—H9B	109.5
C3—C2—H2	119.5	C8—C9—H9C	109.5
C1—C2—H2	119.5	H9A—C9—H9C	109.5
C2—C3—C4	119.49 (15)	H9B—C9—H9C	109.5
C2—C3—H3	120.3	N1—C10—C11	114.87 (13)

C4—C3—H3	120.3	N1—C10—H10A	108.6
C5—C4—C3	120.70 (16)	C11—C10—H10A	108.6
C5—C4—H4	119.7	N1—C10—H10B	108.6
C3—C4—H4	119.7	C11—C10—H10B	108.6
C4—C5—C6	120.41 (16)	H10A—C10—H10B	107.5
C4—C5—H5	119.8	C12—C11—C10	127.48 (17)
C6—C5—H5	119.8	C12—C11—H11	116.3
N1—C6—C5	122.71 (14)	C10—C11—H11	116.3
N1—C6—C1	118.25 (13)	C11—C12—H12A	120.0
C5—C6—C1	119.04 (14)	C11—C12—H12B	120.0
O1—C7—N1	122.11 (14)	H12A—C12—H12B	120.0

C12—C11—C10—N1	−6.7 (3)

Table 1
Offset π–π stacking between the quinoxaline rings.

Cg1 is the centroid of ring N1,C6,C1,N2,C8,C7 and Cg2 the centroid of ring C1–C6.

	Centroid-to-centroid(Å)	plane-to-plane(Å)	offset(°)
Cg1–Cg2^{i}	3.8832 (9)	3.509	25.4

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

Fig. 1

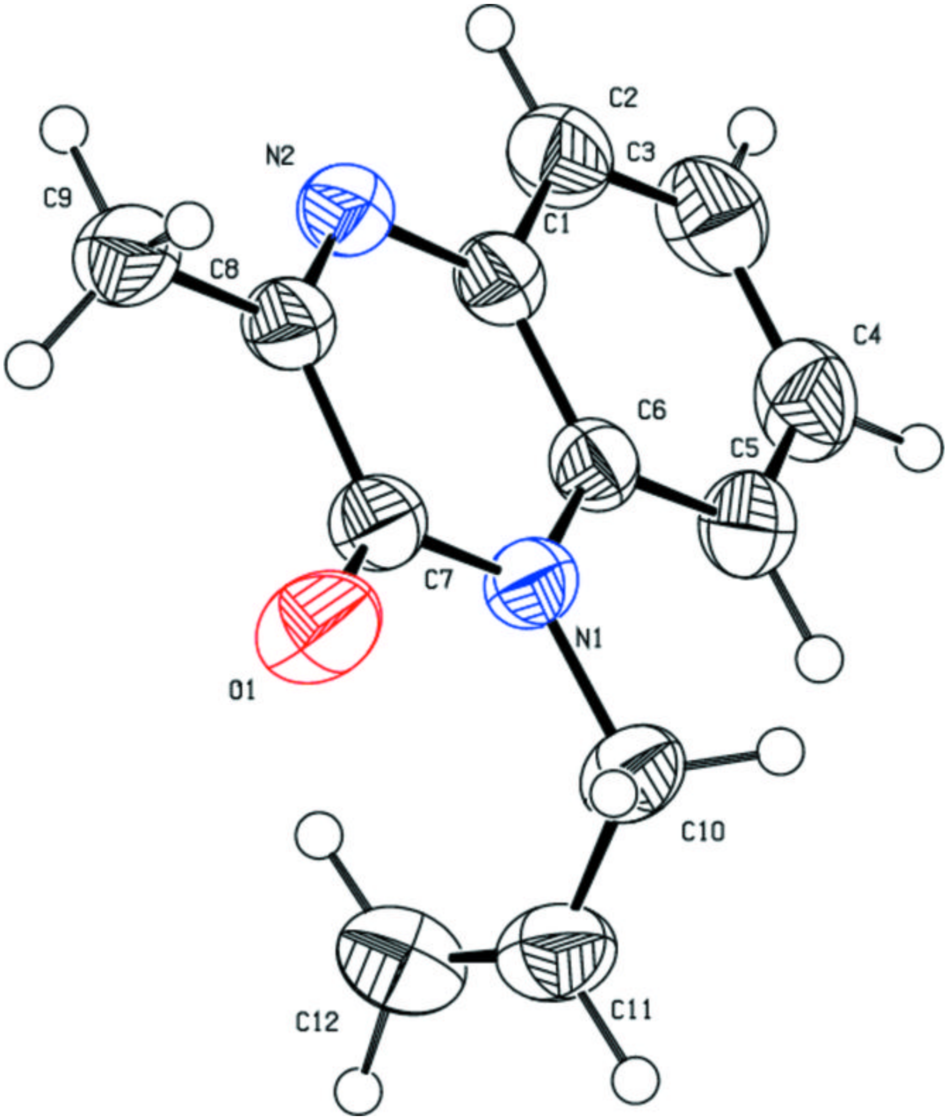

Fig. 2