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## Structure Reports

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

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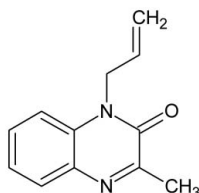
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 Key indicators: single-crystal X-ray study;  $T = 296$  K,  $P = 0.0$  kPa; mean  $\sigma(C-C) = 0.002$  Å;  $R$  factor = 0.051;  $wR$  factor = 0.151; data-to-parameter ratio = 18.5.

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  $\pi$ - $\pi$  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  
 $\beta = 95.082$  (5)°  
 $V = 1024.31$  (17) Å<sup>3</sup>

$Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.32 \times 0.31 \times 0.13$  mm

#### Data collection

Bruker X8 APEXII CCD area-detector diffractometer  
 11850 measured reflections

2546 independent reflections  
 1726 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.049$

#### 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  
 $\Delta\rho_{max} = 0.23$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.17$  e Å<sup>-3</sup>

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).

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

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## supporting information

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

**Youssef Ramli, Rachid Slimani, Hafid Zouihri, Saïd Lazar and E. M. Essassi**

**S1. 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).

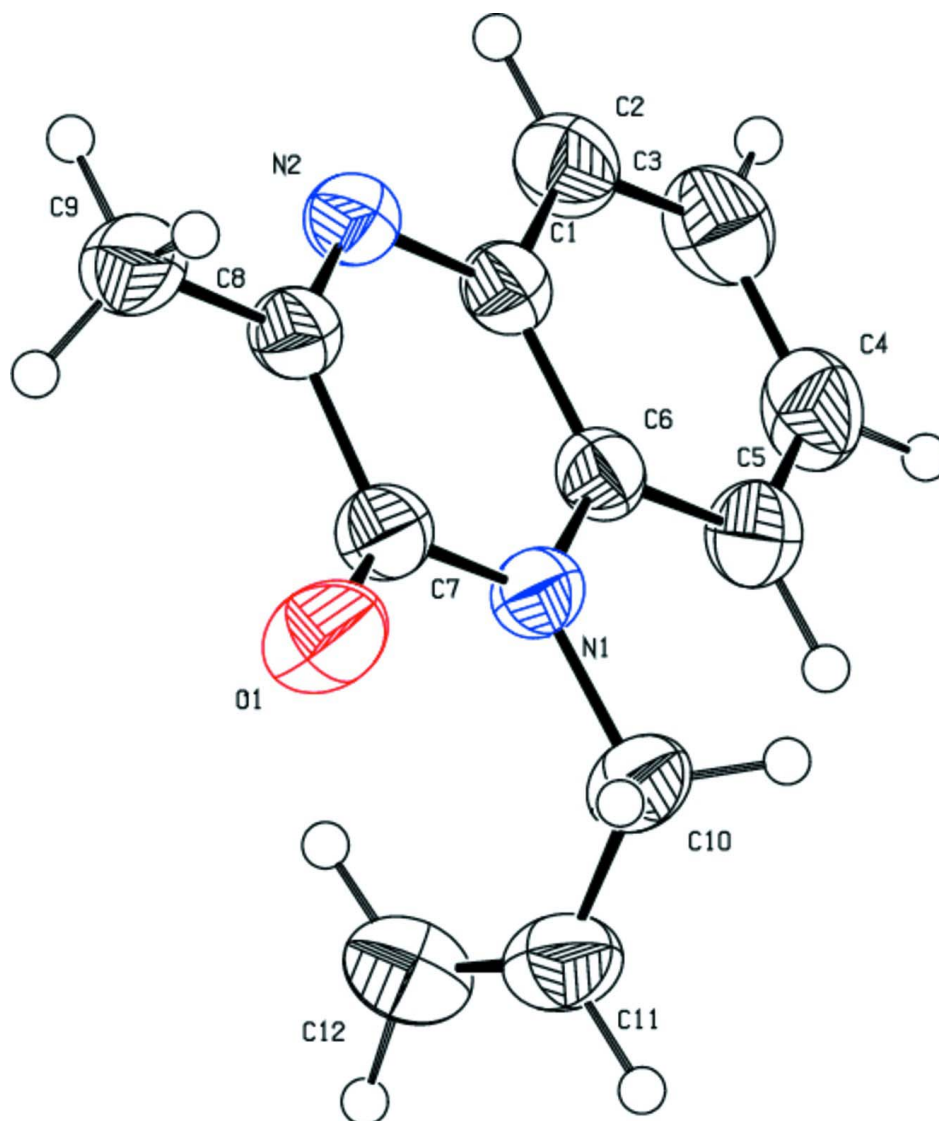
The dihedral angle between the quinoxaline and propenyl planes is 82.1 (2) (Fig. 1). Bond lengths and angles in title molecule are normal (Allen *et al.*, 1987). The crystal packing is stabilized by offset  $\pi$ - $\pi$  stacking between the quinoxalin rings.

**S2. Experimental**

To a solution of 3-methylquinoxali-2(1H)-one (1 g) in 20 ml of dimethylformamide was added allylchloride (0.85 ml), K<sub>2</sub>CO<sub>3</sub> (0.95 g) and catalytic amount of tetrabutylammonium bromide. The mixture was stirred at room temperature for 24 h. Then the solvent was removed under reduced pressure, the residue was crystallized in ethanol to afford the product.

**S3. 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<sub>eq</sub> (aromatic, methine) or U iso (H) = 1.5U<sub>eq</sub> (methyl).

**Figure 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.

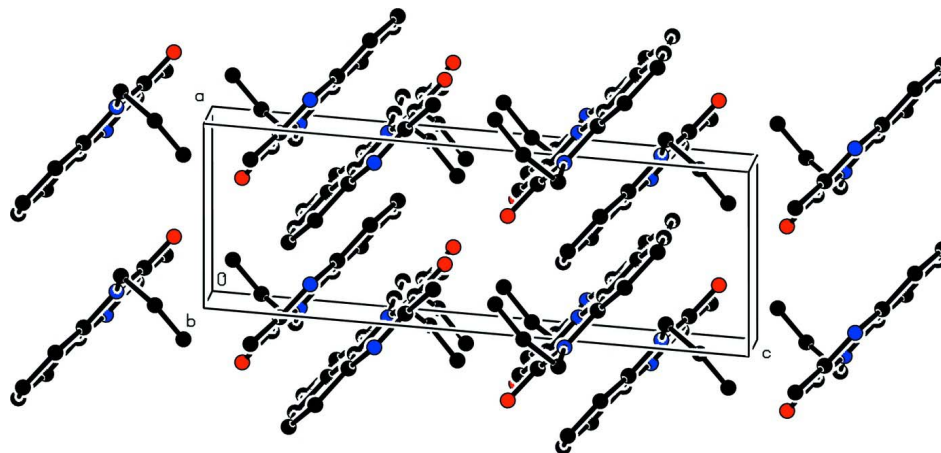


Figure 2

Packing view of the crystal structure of the title compound.

### 3-Methyl-1-(prop-2-en-1-yl)quinoxalin-2(1H)-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<sup>3</sup>

$Z = 4$

$F(000) = 424$

$D_x = 1.298$  Mg m<sup>-3</sup>

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<sup>-1</sup>

$T = 296$  K

Block, colourless

$0.32 \times 0.31 \times 0.13$  mm

#### Data collection

Bruker X8 APEXII CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

11850 measured reflections

2546 independent reflections

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

$R_{int} = 0.049$

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

$h = -6$ → $6$

$k = 0$ → $17$

$l = 0$ → $20$

#### 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  $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.23$  e Å<sup>-3</sup>

$\Delta\rho_{min} = -0.17$  e Å<sup>-3</sup>

*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  $\varphi$  angle for the crystal and each exposure covered  $0.5^\circ$  in  $\omega$  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 estimated using 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 data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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

## supporting information

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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)		

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