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# 2-*p*-Toluoylquinoxaline

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**Key indicators**

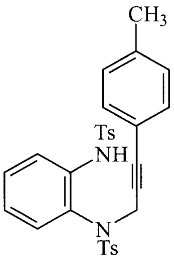
Single-crystal X-ray study
*T* = 293 K
Mean $\sigma$(C–C) = 0.002 Å
*R* factor = 0.043
*wR* factor = 0.127
Data-to-parameter ratio = 19.4

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

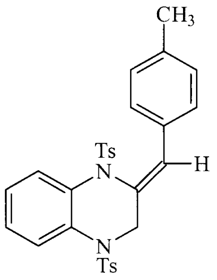
The title compound, $C_{16}H_{12}N_2O$, consists of planar quinoxaline and tolyl moieties linked by a carbonyl group. The carbonyl group is nearly coplanar with the tolyl ring but is inclined at an angle of 34.9 (1)° to the quinoxaline ring. Intermolecular hydrogen bonds stabilize the packing of the molecules in the unit cell.

## Comment

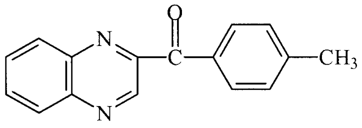
Quinoxaline heterocycles have attracted much attention owing to their natural occurence (Dell *et al.*, 1975) and biological activities (Kher *et al.*, 1995). Many quinoxaline derivatives display unusual solid-tumor selectivity against multidrug-resistant cancer cells (Gao *et al.*, 1999). The synthetic utility and pharmacological importance of these compounds have prompted us to synthesize and characterize novel quinoxaline derivatives (Banerjee *et al.*, 2001). During the synthesis of a di-*p*-tosyl-1,2,3,4-tetrahydroquinoxaline, (II), *via* a palladium–copper catalyzed reaction, an unexpected product, namely 2-*p*-toluoylquinoxaline, (III), was obtained in good yield. The X-ray structure analysis of (III) was undertaken in order to establish the regio- and stereospecificities of the reaction.



(I)



(II)



(III)

The title molecule (Fig. 1) consists of essentially planar quinoxaline and tolyl moieties [the maximum deviation of an in-plane atom from the least-squares plane through the ring atom is 0.032 (1) Å for C2] linked by a carbonyl group. The dihedral angle between the two planar aromatic parts, C1–C8/N1/N2 and C10–C16, is 50.96 (3)°. The carbonyl group is almost coplanar with the tolyl ring [O1—C9—C10—C11 = 15.5 (2)°] but it is inclined at an angle of 34.9 (1)° to the

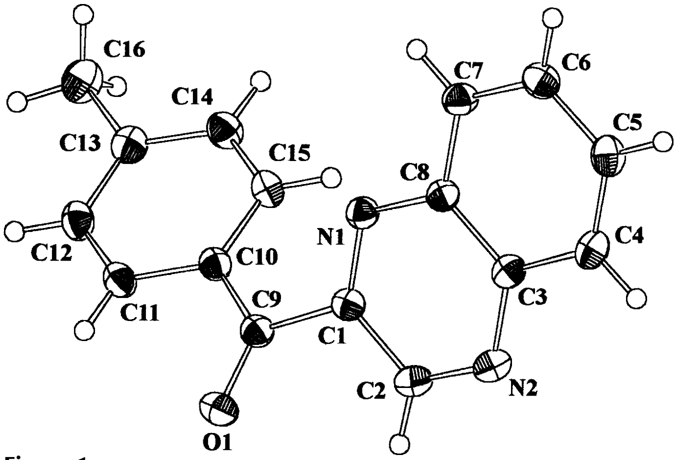


**Figure 1**
*ZORTEP* (Zsolnai, 1995) view (50% probability level) of the molecule of (III).

quinoxaline ring. As a result, the $\pi$ conjugation between the carbonyl group and the tolyl ring is more effective than that for the carbonyl and quinoxaline moieties. This is also reflected in the slight shortening of the C9—C10 bond length [1.489 (2) Å] compared to the C1—C9 distance [1.511 (2) Å]. Other bond distances and angles are comparable to those reported for similar structures (Degen & Bolte, 1999; Fang *et al.*, 2001).

In addition to van der Waals forces, the packing of the molecules in the unit cell is governed by weak C—H···O hydrogen bonds (Table 2).

## Experimental

A mixture of *N*-[(3′-*p*-toluoyl)prop-2′-ynyl]-*N*,*N*′-1,2-phenylenedi-*p*-tosylamide, (I) (1 mmol) (Mukhopadhyay & Kundu, 2000), anhydrous potassium carbonate (2 mmol) and cuprous iodide (10 mol%) in DMF (5 ml) was heated at 373 K for 24 h. After the usual work-up and purification by column chromatography on neutral alumina (10% ethyl acetate in petroleum ether, b.p. 333–353 K, as eluent), 2-*p*-toluoylquinoxaline, (III), was obtained (m.p. 352 K). Single crystals of (III) suitable for X-ray analysis were obtained by slow crystallization from a chloroform–petroleum ether solution. Elemental analysis, calculated for $C_{16}H_{12}N_2O$: C 77.41, H 4.83, N 11.29%; found: C 77.07, H 5.00, N 10.95%.

*Crystal data*

$C_{16}H_{12}N_2O$
$M_r = 248.28$
Monoclinic, $P2_1/n$
$a = 5.5973$ (2) Å
$b = 18.5701$ (5) Å
$c = 11.8195$ (3) Å
$\beta = 91.304$ (1)°
$V = 1228.23$ (6) Å$^3$
$Z = 4$

$D_x = 1.343$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 918 reflections
$\theta = 5.1$–$31.0°$
$\mu = 0.09$ mm$^{-1}$
$T = 293$ (2) K
Block, yellow
0.55 × 0.50 × 0.30 mm

*Data collection*

Bruker SMART–CCD diffractometer
$\omega$ scans
9672 measured reflections
3352 independent reflections
2864 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.028$
$\theta_{\rm max} = 29.8°$
$h = -7 \rightarrow 7$
$k = -25 \rightarrow 25$
$l = -16 \rightarrow 12$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.127$
$S = 1.04$
3352 reflections
173 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0718P)^2 + 0.3457P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.38$ e Å$^{-3}$
$\Delta\rho_{\rm min} = -0.20$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C1—N1 | 1.3203 (14) | C9—O1 | 1.2243 (14) |
| C1—C9 | 1.5108 (15) | C9—C10 | 1.4888 (15) |
| C2—N2 | 1.3158 (15) | | |
| O1—C9—C10 | 121.53 (10) | C1—N1—C8 | 116.21 (9) |
| O1—C9—C1 | 117.57 (10) | C2—N2—C3 | 116.30 (9) |
| C10—C9—C1 | 120.91 (9) | | |
| C2—C1—C9—O1 | 34.89 (14) | O1—C9—C10—C11 | 15.52 (15) |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···O1$^{\rm i}$ | 0.93 | 2.70 | 3.4611 (14) | 140 |
| C6—H6···O1$^{\rm ii}$ | 0.93 | 2.62 | 3.4155 (14) | 144 |
| C11—H11···O1$^{\rm iii}$ | 0.93 | 2.59 | 3.4650 (14) | 158 |

Symmetry codes: (i) $1 - x, -y, 1 - z$; (ii) $\frac{1}{2} + x, \frac{1}{2} - y, z - \frac{1}{2}$; (iii) $-x, -y, 1 - z$.

The structure was solved by direct methods using *MULTAN*88 (Debaerdemaeker *et al.*, 1988). The H atoms were refined using a riding model and their isotropic displacement parameters were set to 1.2 times (1.5 times for $CH_3$ groups) the equivalent displacement parameters of their parent atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *MULTAN*88 (Debaerdemaeker *et al.*, 1988); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1995).

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