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2-Phenyl-4-(*p*-toluidinomethylene)-5-oxazolone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.125
Data-to-parameter ratio = 13.5

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

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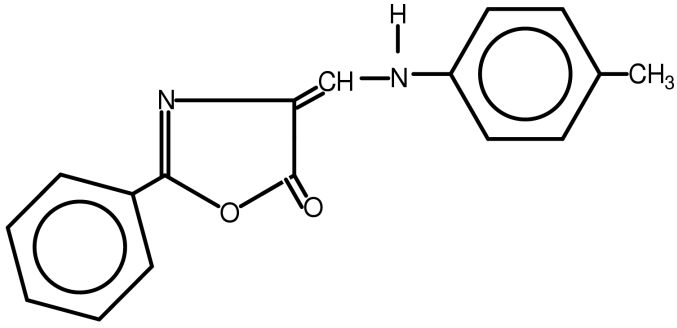
The two crystallographically independent molecules in the asymmetric unit of the title compound, $C_{17}H_{14}N_2O_2$, have nearly the same molecular geometry. The planarity of the oxazoline ring is not affected by substitutions at the 2 and 4 positions. The structure is stabilized by N—H···O type intermolecular interactions.

Comment

The structure determination of the title compound, (I), was undertaken to study the effect of substitutions at the 2 and 4 positions on the oxazoline ring and the nature of hydrogen bonding. There are two crystallographically independent molecules in the asymmetric unit, Molecules I and II (atoms are labelled with addition letter *A* to the corresponding atoms of molecule II). The planarity of the oxazoline ring is not affected by the substitutions on the 2 and 4 positions. The dihedral angle between the phenyl ring and the oxazoline ring is 17.29 (10)° [13.35 (10)°]. The dihedral angle between the oxazoline ring and the toluidino moiety is 26.68 (10)° [19.10 (9)°]. The N7—C6 bond {1.329 (2) Å [1.322 (2) Å]} shows a partial double-bond character. This may be due to the delocalization of the lone pair of electrons of the N atom over the N7—C6═C4 moiety (Thiruvalluvar & Parthasarathi, 1995). The exocyclic bond angles N3—C2—C15 and N3*A*—C2*A*—C15*A* are 128.0 (2) and 128.1 (2)°, respectively. This increase from the normal 120° may be the consequence of the repulsion between the lone pair of electrons of the N and the H atom of C20 and C20*A* (Vijayalakshmi *et al.*, 1998). In the crystal, the N—H groups of the molecules are involved in N—H···O type intermolecular hydrogen bonds (Table 2).



(I)

Experimental

Triethylorthoformate (3.32 ml, 20 mmol) and acetic anhydride (3.57 ml, 38 mmol) were added to *N*-benzoylglycine (3.580 g, 20 mmol). The resulting reaction mixture was refluxed for 30 min and

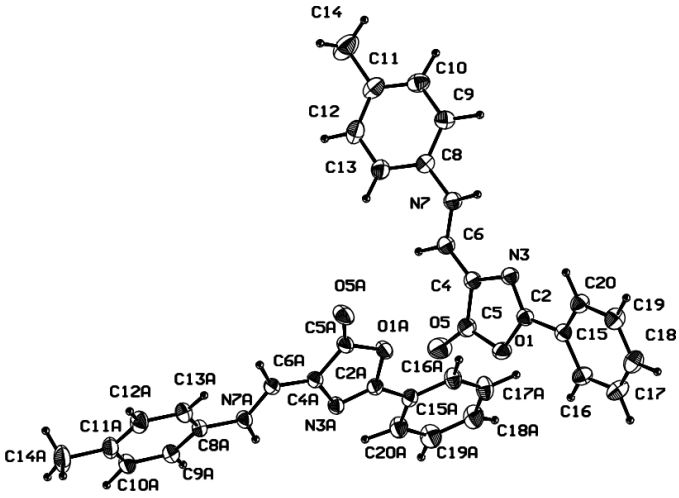


Figure 1
The molecular structure of (I) showing 30% probability displacement ellipsoids.

then kept in a freezer overnight. The precipitate of 4-(ethoxymethylene)-2-phenyl-5-oxazolone was filtered and washed with petroleum ether and dried. Equimolar quantities of 4-(ethoxymethylene)-2-phenyl-5-oxazolone and *p*-toluidine were taken in 10 ml of ethanol and the reaction mixture was refluxed for 2 h. On cooling, a precipitate of (I) was obtained, which was washed with petroleum ether and ethanol and then recrystallized from ethanol.

Crystal data

$C_{17}H_{14}N_2O_2$	D_x = 1.283 Mg m^{-3}
M_r = 278.30	Cu Kα radiation
Monoclinic, $P2_1/a$	Cell parameters from 25 reflections
a = 19.457 (2) Å	θ = 25–35°
b = 6.442 (1) Å	μ = 0.69 mm^{-1}
c = 24.619 (1) Å	T = 293 (2) K
β = 110.95 (8)°	Plate, green
V = 2882.1 (5) Å^3	0.30 × 0.15 × 0.10 mm
Z = 8	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.014
ω–2θ scans	θ_{max} = 68.0°
Absorption correction: ψ scan (North *et al.*, 1968)	$h = -22 \rightarrow 21$
T_{min} = 0.977, T_{max} = 0.999	$k = 0 \rightarrow 7$
5422 measured reflections	$l = 0 \rightarrow 29$
5130 independent reflections	2 standard reflections
4460 reflections with $I > 2\sigma(I)$	frequency: 120 min
	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 0.9752P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.125	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
S = 1.06	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
5130 reflections	Extinction correction: *SHELXL*97
380 parameters	Extinction coefficient: 0.0016 (1)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N3—C2	1.277 (2)	N3*A*—C2*A*	1.282 (2)
N3—C4	1.400 (2)	N3*A*—C4*A*	1.402 (2)
N7—C8	1.417 (2)	N7*A*—C8*A*	1.416 (2)
C4—C6	1.362 (2)	C4*A*—C6*A*	1.370 (2)
C8—N7—C6—C4	−178.7 (2)	C8*A*—N7*A*—C6*A*—C4*A*	180.0 (2)
C6—N7—C8—C13	23.7 (3)	C6*A*—N7*A*—C8*A*—C13*A*	−20.9 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7···O5^{i}	0.95	1.91	2.822 (2)	161
N7*A*—H7*A*···O5*A*^{ii}	0.92	1.98	2.809 (2)	151

Symmetry codes: (i) $x, 1 + y, z$; (ii) $x, y - 1, z$.

All but methyl group H atoms were located from the difference map and were included in the structure-factor calculations with isotropic displacement parameters equal to 1.1U_{eq} of their respective carrier atom, but their positional parameters were not refined (C—H distances are in the range 0.95–1.10 Å), whereas the methyl H atoms were geometrically fixed and a riding model was used for their refinement.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997); software used to prepare material for publication: *SHELXL*97.

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