Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Benzoyl-3-methyl-4-benzylidenamino-4,5-dihydro-1,2,4-triazol-5-one

Tuncay Karakurt,[a]* Muharrem Dinçer,[a] Bahittin Kahveci,[b] Erbil Ağar,[c] Ayşen Ağar[c] and Selami Şaşmaz[d]

[a]Ondokuz Mayıs University, Arts and Sciences Faculty, Department of Physics, 55139 Samsun, Turkey, [b]Karadeniz Teknik University, Rize Arts and Sciences Faculty, Department of Chemistry, 55139 Sanmsun, Turkey, [c]Ondokuz Mayıs University, Arts and Sciences Faculty, Department of Chemistry, 55139 Samsun, Turkey, and [d]Karadeniz Teknik University, Rize Arts and Sciences Faculty, Department of Chemistry, Rize, Turkey

Correspondence e-mail: mdincer@omu.edu.tr

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.096
Data-to-parameter ratio = 10.2

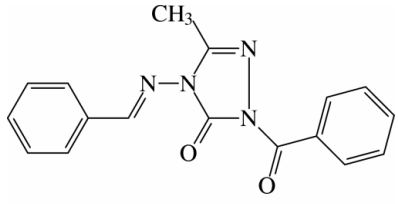
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 5 September 2003
Accepted 24 September 2003
Online 7 October 2003

In the title molecule, $C_{17}H_{14}N_4O_2$, the benzylidenamino group is almost coplanar with the triazole ring. The dihedral angle between the triazole ring and the benzoyl phenyl ring is 58.74 (8)°. The molecular structure is stabilized by a C—H···O hydrogen bond and the crystal structure is stabilized by intermolecular C—H···O and C—H...π interactions.

Comment

The discovery of a unique property of 1,2,4-triazole derivatives, *viz.* the inhibition of the biosynthesis of ergosterins, has stimulated an intensive search for new active compounds (Mel'nikov & Mil'shtein, 1986). 1,2,4-Triazoles are also very useful ligands in coordination chemistry (Bencini *et al.*, 1985, 1987; van Koningsbruggen *et al.*, 1995). Furthermore, condensed 1,2,4-triazoles are biologically important compounds (Kottke *et al.*, 1993; Francis & Gelette, 1988; Francis *et al.*, 1988). A large number of heterocyclic compounds containing the 1,2,4-triazole ring are associated with diverse pharmacological properties, such as anti-inflammatory, fungicidal, antimicrobial and antiviral activity (Walser *et al.*, 1991; Todoulou *et al.*, 1994). Therefore, the crystal structure determination of the title compound, (I), was carried out.



(I)

The title molecule (Fig. 1) contains three rings, a triazole ring (*A*) and two phenyl rings *B* (C1–C6) and *C* (C12–C17). The bond lengths and angles in (I) are normal (Table 1). The triazole ring is planar and the benzylidenamino group is almost coplanar with it [C8—N3—N4—C11 −175.56 (14)°, N3—N4—C11—C12 179.74 (13)°, N4—C11—C12—C17 −172.79 (17)°]. The dihedral angle between the triazole ring and phenyl ring *C* is 12.38 (10)°. The benzoyl phenyl ring *B* forms a dihedral angle of 58.74 (8)° with ring *A*. The molecular and crystal structures are stabilized by C—H···O and C—H···π interactions (Table 2). A view of the molecular packing is shown in Fig. 2.

Experimental

The corresponding Schiff base (3-methyl-4-benzylideneamino-4,5-dihydro-1*H*-1,2,4-triazol-5-one; 1.01 g, 0.005 mol) in a round-

bottomed flask was dissolved in 25 ml NaOH (5%) (Kahveci & İkizler, 2000). To this benzoyl chloride (0.64 ml) was added dropwise and the closed reaction vessel was shaken for 0.5 h at room temperature. The product was obtained by filtration, washed with water, dried and recrystallized from ethanol. Yield: 78.60%.

Crystal data

$C_{17}H_{14}N_4O_2$	D_x = 1.331 Mg m^{-3}
M_r = 306.32	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 9403 reflections
a = 28.850 (4) Å	θ = 2.9–29.4°
b = 7.4438 (5) Å	μ = 0.09 mm^{-1}
c = 15.3364 (19) Å	T = 293 (2) K
β = 111.853 (10)°	Prism, colourless
V = 3056.9 (6) Å^3	0.73 × 0.52 × 0.30 mm
Z = 8	

Data collection

Stoe IPDS 2 diffractometer	R_{int} = 0.072
φ scans	θ_{max} = 25.0°
Absorption correction: none	$h = -39 \rightarrow 39$
4262 measured reflections	$k = -10 \rightarrow 9$
2700 independent reflections	$l = -20 \rightarrow 21$
1899 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0712P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.038	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.096	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
S = 0.87	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
2700 reflections	Extinction correction: *SHELXL*97
265 parameters	Extinction coefficient: 0.0073 (6)
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.2008 (17)	N3—N4	1.3863 (16)
O2—C9	1.2029 (17)	N3—C9	1.3967 (18)
N1—C9	1.3890 (18)	N4—C11	1.260 (2)
N1—N2	1.3955 (16)	C1—C7	1.475 (2)
N1—C7	1.4179 (18)	C8—C10	1.474 (2)
N3—C8	1.3708 (18)	C11—C12	1.467 (2)
C9—N1—C7	127.37 (12)	N1—C7—C1	114.84 (12)
N2—N1—C7	119.74 (11)	N2—C8—C10	125.23 (14)
C8—N3—N4	119.59 (11)	N3—C8—C10	123.22 (13)
N4—N3—C9	130.59 (12)	O2—C9—N1	130.04 (13)
C11—N4—N3	119.34 (12)	O2—C9—N3	128.80 (13)
O1—C7—N1	120.33 (13)	N4—C11—C12	118.75 (15)
O1—C7—C1	124.83 (13)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H6···O2	0.96 (2)	2.29 (2)	2.932 (2)	124 (1)
C5—H13···O1^{i}	1.02 (2)	2.55 (2)	3.320 (2)	132 (2)
C5—H13···O2^{i}	1.02 (2)	2.56 (2)	3.525 (2)	157 (2)
C17—H1···$Cg1^{ii}$	1.00 (2)	2.89 (2)	3.537 (2)	123 (2)
C14—H4···$Cg2^{iii}$	1.00 (3)	2.93 (3)	3.684 (3)	132 (2)
C10—H7···$Cg1^{iv}$	0.99 (3)	2.87 (2)	3.644 (2)	136 (2)
C2—H10···$Cg2^{v}$	0.99 (2)	2.92 (2)	3.527 (2)	120 (1)

Symmetry codes: (i) $x, 1-y, \frac{1}{2}+z$; (ii) $-x, 1-y, -z$; (iii) $-\frac{1}{2}-x, y-\frac{1}{2}, -\frac{1}{2}-z$; (iv) $-x, y, \frac{1}{2}-z$; (v) $-x, -y, -z$. $Cg1$ and $Cg2$ denote the centroids of the rings B and C, respectively.

All H atoms were located in a difference Fourier map and their positional and isotropic displacement parameters were refined. The C—H bond lengths are in the range 0.94 (2)–1.03 (2) Å and the U_{iso} values lie in the range 0.063 (4)–0.154 (10) Å^2.

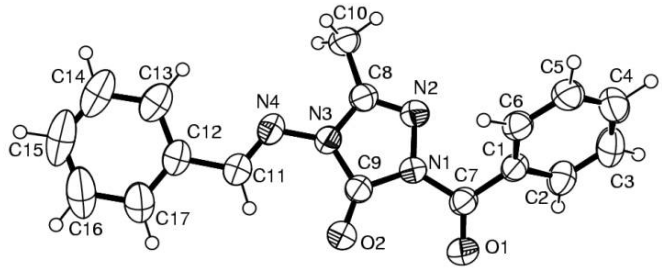


Figure 1
An *ORTEP*III (Farrugia, 1997) plot of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

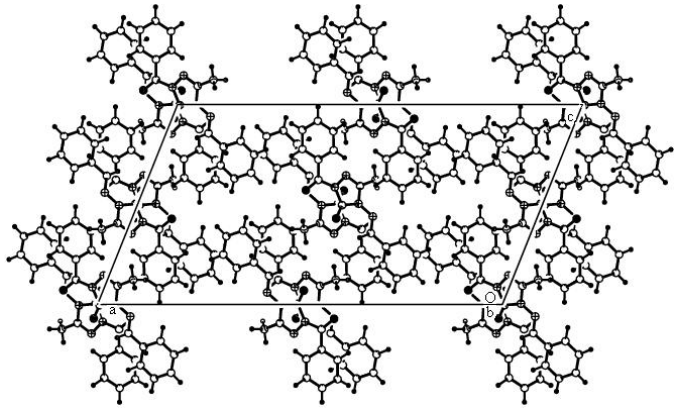


Figure 2
The molecular packing, viewed down the *b* axis.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *PLATON* (Spek, 1990); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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