Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

6-Phenyl-4,5-dihydropyridazin-3(2*H*)-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.098
Data-to-parameter ratio = 12.2

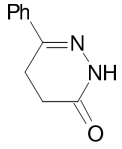
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 30 April 2003
Accepted 7 May 2003
Online 16 May 2003

The title compound, $C_{10}H_{10}N_2O$, is of pharmacological interest. It contains a keto-tetrahydropyridazine ring carrying a phenyl ring *para* to the carbonyl group. In the crystal structure, hydrogen-bonded centrosymmetric dimers are observed.

Comment

Pyridazine compounds homologous to the title compound, (I), are known and are of particular interest as antidepressive agents (Biziere *et al.*, 1988). This kind of compound has also been used for the treatment of Alzheimer's disease (Passeri *et al.*, 1985).



(I)

The geometric parameters of (I) are normal. The dihydropyridazine ring adopts a half-chair conformation, with atoms C1, N2, N3 and C4 in a common plane and C5 0.222 (2) Å and C6 0.262 (2) Å on opposite sides of this plane. The plane is almost coplanar with the phenyl ring; the dihedral angle between the two planes is 1.73 (9) Å. In the crystal structure, hydrogen-bonded centrosymmetric dimers are observed.

Experimental

142.4 g (8 mmol) of benzoylpropionic acid was dissolved in 170 ml ethanol. 43 g (8.6 mmol) of hydrazine hydrate was then added to this mixture and it was refluxed for 1 h. After cooling to room temperature, yellow crystals grew from the solution and were filtered off and dried.

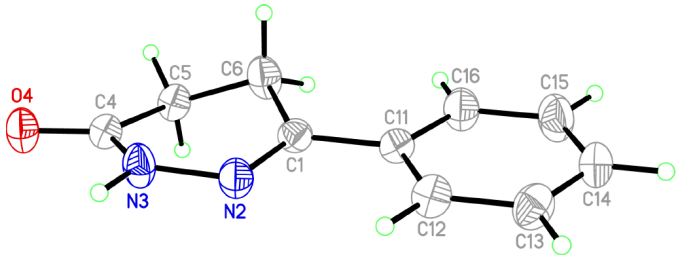


Figure 1
Perspective view of the asymmetric unit of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Crystal data

$C_{10}H_{10}N_2O$
$M_r = 174.20$
Triclinic, $P\overline{1}$
$a = 5.6712\ (10)$ Å
$b = 8.1749\ (14)$ Å
$c = 10.1055\ (17)$ Å
$\alpha = 104.740\ (14)^\circ$
$\beta = 104.392\ (13)^\circ$
$\gamma = 98.097\ (14)^\circ$
$V = 428.33\ (13)$ Å^3
$Z = 2$
$D_x = 1.351$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10040 reflections
$\theta = 3.7$–25.1°
$\mu = 0.09$ mm^{-1}
$T = 173\ (2)$ K
Block, colourless
0.44 × 0.38 × 0.36 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: none
5318 measured reflections
1483 independent reflections
1318 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0^\circ$
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 9$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.098$
$S = 1.08$
1483 reflections
122 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2 + 0.0435P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N2	1.2830 (15)	N3—C4	1.3464 (15)
N2—N3	1.3877 (14)	C4—O4	1.2316 (14)
C1—N2—N3	117.98 (9)	C4—N3—N2	127.23 (9)
C1—N2—N3—C4	15.45 (18)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O4^{i}	0.870 (16)	1.990 (16)	2.8587 (13)	177.1 (14)

Symmetry code: (i) $1-x, 1-y, 2-z$.

H atoms bonded to C atoms were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C)], using a riding model with aromatic C—H = 0.99 Å and methylene C—H = 0.98 Å. The H atom bonded to N was refined freely.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97.

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