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Crystal Structure
Communications

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5-Amino-6-phenyl-1,6-dihydro-
pyridazin-3(2H)-oneHéctor Novoa de Armas,^{a,†} Norbert M. Blaton,^a
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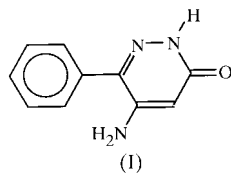
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In the title compound, C₁₀H₉N₃O, the pyridazinone moiety is essentially planar and forms a dihedral angle of 49.5 (1)° with the phenyl substituent. The molecular packing is stabilized by van der Waals interactions and hydrogen bonds.

Comment

It is known that 6-aryl-3(2H)-pyridazinones and their 4,5-dihydro derivatives display several pharmacological activities, all of them related to cardiotonics, such as reduction of blood pressure, inhibition of platelet aggregation, positive inotropic activity, and others (Robertson *et al.*, 1986). Likewise, 6-aryl-pyridazinones with nitro and acyl substituents at the 4- and 5-positions show good antiaggregating properties (Schudt *et al.*, 1991). We have previously reported the synthesis of 5-aminomethyl-6-aryl-4,5-dihydropyridazinones and 6-aryl-5-aminomethyl-3(2H)-pyridazinones (Raviña *et al.*, 1990). Some of these compounds show a good *in vitro* inhibitory activity on ADP-induced rat platelet aggregation. As a continuation of this previous report on the chemistry and pharmacology of this class of compounds, we carried out the crystal structure



determination of 5-amino-6-phenyl-1,6-dihydropyridazin-3(2H)-one, (I). This enamine-like compound can be employed in the synthesis of hetero-condensed pyridazinones. Recently,

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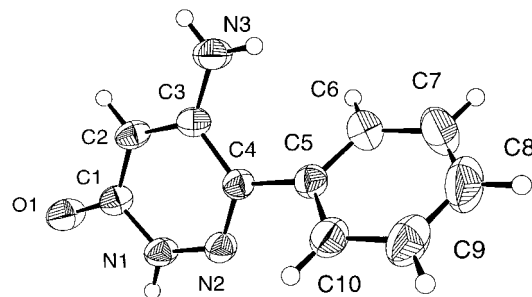


Figure 1

A plot of (I) showing the atomic numbering scheme. Displacement ellipsoids are drawn at 50% probability level, and H atoms are shown as spheres of arbitrary radii.

we used this compound as an intermediate in the synthesis of pyrido[2,3-*d*]pyridazines (Pita *et al.*, 2000).

There are no unusual bond distances and angles in (I), and they are in the range of calculated values using the *AM1* method in related structures (Estevez *et al.*, 1998). The bond lengths in the pyridazinone ring range from 1.304 (2) to 1.450 (3) Å. The torsion angle between the pyridazinone and the phenyl ring, found using the quantum chemical *AM1* method in *MOPAC* (Stewart, 1990) for the lower energy conformations, is in the range 40–140°, with a heat of formation of 38.30 kcal mol⁻¹ (1 kcal = 4.184 kJ). In the crystal structure this angle is -51.3 (3)°, which corresponds to the minimum in the energy calculations. The calculated favoured conformation of the enol form corresponds to torsion angles in the same range (40–140°) and a heat of formation of 34.20 kcal mol⁻¹, which shows that this enol is the predominant form at equilibrium. This is contrary to the fact that in the crystal the molecule is present in the amide form, which corresponds to a higher heat of formation. The dihedral angle between the respective least-squares planes of the pyridazinone ring and the phenyl ring is 49.5 (1)°. The mean Csp²—Csp² bond length within the phenyl ring is 1.382 (1) Å. A view of (I) can be seen in Fig. 1.

The N3 atom of the amine and the N1 atom of the amide group in the pyridazinone ring are involved in two intermolecular hydrogen bonds with a neighbouring O1, forming an infinite two-dimensional network in the plane [001].

Experimental

A suspension of 5-bromo-6-phenyl-3(2H)-pyridazinone (0.5 g, 1.9 mmol), ammonium chloride (0.3 g, 5.6 mmol) and ammonium hydroxide (50 ml) was heated at 458 K at pressure of 374 psi (1 psi ≈ 6.895 kPa) for 3 h in a Parr reactor. The mixture was evaporated *in vacuo* and washed with ammonium hydroxide, and the solid obtained, (I), was recrystallized from ethanol (yield 70%; m.p. 517 K). Spectroscopic analysis: IR (KBr), cm⁻¹: 3480–3425 (NH), 1670 (CO); ¹H NMR (DMSO-*d*₆, p.p.m.): δ 12.12 (*s*, 1H, NH, deuterium oxide exchangeable), 7.50–7.43 (*m*, 5H, aromatics), 5.71 (*s*, 1H, CH—CO), 5.96 (*s*, 2H, NH₂); ¹³C NMR (p.p.m.): δ 162.5 (C3), 99.1 (C4), 149.2 (C5), 140.1 (C6), 134.4 (C1'), 129.1 (C2', C6'), 128.8 (C3', C5'), 129.1 (C4'); analysis, calculated: C 64.16, H 4.85, N 22.45%; found: C 64.20, H 4.78, N 22.43%.

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.265 (2)	N3—C3	1.346 (3)
N1—N2	1.344 (2)	C1—C2	1.395 (3)
N1—C1	1.367 (2)	C2—C3	1.376 (3)
N2—C4	1.304 (2)	C3—C4	1.450 (3)
N2—N1—C1	125.86 (15)	N3—C3—C2	122.12 (17)
N1—N2—C4	118.06 (15)	N3—C3—C4	120.82 (16)
O1—C1—C2	126.04 (17)	N2—C4—C5	114.71 (16)
N1—C1—C2	115.88 (16)	N2—C4—C3	121.97 (16)
O1—C1—N1	118.07 (16)		

Crystal data

C₁₀H₉N₃O
M_r = 187.20
Orthorhombic, *Pbca*
a = 8.752 (2) Å
b = 10.525 (5) Å
c = 20.619 (5) Å
V = 1899.3 (11) Å³
Z = 8
D_x = 1.309 Mg m⁻³

Cu Kα radiation
Cell parameters from 25 reflections
θ = 10.78–28.12°
μ = 0.73 mm⁻¹
T = 293 (2) K
Prism, light green
0.48 × 0.20 × 0.14 mm

Data collection

Siemens P4 four-circle diffractometer
2θ/ω scans
Absorption correction: ψ-scan (North *et al.*, 1968)
T_{min} = 0.626, T_{max} = 0.903
1733 measured reflections
1266 independent reflections
1102 reflections with I > 2σ(I)

R_{int} = 0.024
θ_{max} = 57.19°
h = -1 → 9
k = -1 → 11
l = -1 → 22
3 standard reflections every 100 reflections
intensity decay: <1.0%

Refinement

Refinement on F²
R(F) = 0.038
wR(F²) = 0.104
S = 1.100
1266 reflections
128 parameters
H-atom parameters constrained

w = 1/[σ²(F_o²) + (0.0532P)² + 0.757P]
where P = (F_o² + 2F_c²)/3
(Δ/σ)_{max} = 0.002
Δρ_{max} = 0.14 e Å⁻³
Δρ_{min} = -0.14 e Å⁻³
Extinction correction: SHELXL97 (Sheldrick, 1997)
Extinction coefficient: 0.0110 (8)

Data collection: XSCANS (Siemens, 1996); cell refinement: XSCANS; data reduction: XSCANS; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97; molecular graphics: DIAMOND (Bergerhoff, 1996); software used to prepare material for publication: PLATON

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

D—H...A	D—H	H...A	D...A	D—H...A
N1—H1...O1 ⁱ	0.86	1.96	2.818 (2)	180
N3—H3A...O1 ⁱⁱ	0.86	2.06	2.880 (3)	159

Symmetry codes: (i) -x, -y, -z; (ii) ½ + x, ½ - y, -z.

(Spek, 1990), PARST (Nardelli, 1983, 1995) and PARSTCIF (Nardelli, 1992).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1336). Services for accessing these data are described at the back of the journal.

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supporting information

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5-Amino-6-phenyl-1,6-dihydropyridazin-3(2H)-one

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Computing details

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997b); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *DIAMOND* (Bergerhoff, 1996); software used to prepare material for publication: *PLATON* (Spek, 1990), *PARST* (Nardelli, 1983, 1995) and *PARSTCIF* (Nardelli, 1992).

5-Amino-6-phenyl-1,6-dihydropyridazin-3(2H)-one

Crystal data

C₁₀H₉N₃O

$M_r = 187.20$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 8.752(2) \text{ \AA}$

$b = 10.525(5) \text{ \AA}$

$c = 20.619(5) \text{ \AA}$

$V = 1899.3(11) \text{ \AA}^3$

$Z = 8$

$F(000) = 784$

$D_x = 1.309 \text{ Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$

Cell parameters from 25 reflections

$\theta = 10.8\text{--}28.1^\circ$

$\mu = 0.73 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Prism, light green

$0.48 \times 0.20 \times 0.14 \text{ mm}$

Data collection

Siemens P4 four-circle
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$2\theta/\omega$ scans

Absorption correction: ψ -scan
(North et al., 1968)

$T_{\min} = 0.626$, $T_{\max} = 0.903$

1733 measured reflections

1266 independent reflections

1102 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 57.2^\circ$, $\theta_{\min} = 4.3^\circ$

$h = -1 \rightarrow 9$

$k = -1 \rightarrow 11$

$l = -1 \rightarrow 22$

3 standard reflections every 100 reflections

intensity decay: $<1.0\%$

Refinement

Refinement on F^2

Least-squares matrix: Full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.104$

$S = 1.10$

1266 reflections

128 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

$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2 + 0.757P]$

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

$$(\Delta/\sigma)_{\max} = 0.002$$

$$\Delta\rho_{\max} = 0.14 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.14 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick, 1997a), $F_c^* = kF_c [1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0110 (8)

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All e.s.d.'s are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. The structure was solved by direct methods and Fourier synthesis. Non-H atoms were refined anisotropically by full-matrix least-squares techniques.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.11598 (15)	0.12824 (13)	0.02499 (7)	0.0510 (5)
N1	0.17603 (17)	-0.02452 (14)	-0.04753 (7)	0.0394 (5)
N2	0.26660 (17)	-0.08609 (15)	-0.08973 (7)	0.0385 (5)
N3	0.59357 (19)	0.12476 (17)	-0.08433 (9)	0.0503 (6)
C1	0.2131 (2)	0.08360 (17)	-0.01433 (9)	0.0361 (6)
C2	0.3567 (2)	0.13477 (17)	-0.02767 (9)	0.0375 (6)
C3	0.4539 (2)	0.07773 (17)	-0.07128 (9)	0.0348 (6)
C4	0.4014 (2)	-0.03863 (17)	-0.10159 (8)	0.0346 (6)
C5	0.4959 (2)	-0.11395 (19)	-0.14795 (9)	0.0387 (6)
C6	0.5656 (3)	-0.0585 (2)	-0.20123 (10)	0.0550 (8)
C7	0.6450 (3)	-0.1341 (3)	-0.24540 (12)	0.0736 (10)
C8	0.6569 (3)	-0.2625 (3)	-0.23604 (13)	0.0767 (10)
C9	0.5887 (3)	-0.3180 (3)	-0.18367 (12)	0.0635 (9)
C10	0.5084 (2)	-0.2448 (2)	-0.13948 (10)	0.0481 (7)
H1	0.08672	-0.05595	-0.04081	0.0512*
H2	0.38729	0.20876	-0.00671	0.0487*
H3A	0.62458	0.19259	-0.06515	0.0654*
H3B	0.65179	0.08699	-0.11184	0.0654*
H6	0.55937	0.02884	-0.20754	0.0715*
H7	0.69038	-0.09698	-0.28152	0.0957*
H8	0.71141	-0.31196	-0.26538	0.0999*
H9	0.59621	-0.40536	-0.17765	0.0826*
H10	0.46255	-0.28333	-0.10386	0.0626*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0381 (8)	0.0439 (9)	0.0709 (10)	-0.0002 (6)	0.0115 (7)	-0.0187 (7)
N1	0.0320 (9)	0.0355 (10)	0.0506 (9)	-0.0025 (7)	0.0050 (7)	-0.0081 (7)
N2	0.0359 (9)	0.0363 (9)	0.0432 (9)	-0.0014 (7)	0.0036 (7)	-0.0069 (7)
N3	0.0392 (10)	0.0461 (11)	0.0657 (12)	-0.0100 (8)	0.0110 (8)	-0.0147 (9)
C1	0.0352 (10)	0.0274 (10)	0.0458 (11)	0.0048 (8)	-0.0012 (8)	-0.0030 (8)
C2	0.0359 (10)	0.0268 (10)	0.0498 (11)	-0.0001 (8)	-0.0026 (9)	-0.0050 (8)
C3	0.0329 (10)	0.0302 (10)	0.0412 (10)	0.0002 (8)	-0.0019 (8)	0.0031 (8)
C4	0.0363 (11)	0.0315 (11)	0.0361 (10)	-0.0006 (8)	-0.0001 (8)	-0.0008 (8)

C5	0.0345 (10)	0.0429 (12)	0.0388 (10)	-0.0018 (9)	-0.0005 (8)	-0.0050 (9)
C6	0.0555 (13)	0.0609 (14)	0.0485 (12)	-0.0034 (12)	0.0095 (10)	-0.0031 (11)
C7	0.0655 (16)	0.100 (2)	0.0552 (14)	-0.0064 (15)	0.0222 (12)	-0.0095 (15)
C8	0.0595 (16)	0.096 (2)	0.0746 (18)	0.0097 (15)	0.0132 (13)	-0.0373 (16)
C9	0.0577 (14)	0.0575 (15)	0.0754 (16)	0.0120 (12)	-0.0010 (13)	-0.0252 (13)
C10	0.0478 (12)	0.0457 (13)	0.0508 (12)	-0.0003 (10)	0.0003 (9)	-0.0097 (10)

Geometric parameters (Å, °)

O1—C1	1.265 (2)	C5—C10	1.393 (3)
N1—N2	1.344 (2)	C5—C6	1.385 (3)
N1—C1	1.367 (2)	C6—C7	1.395 (4)
N2—C4	1.304 (2)	C7—C8	1.369 (4)
N3—C3	1.346 (3)	C8—C9	1.365 (4)
N1—H1	0.8600	C9—C10	1.385 (3)
N3—H3A	0.8601	C2—H2	0.9300
N3—H3B	0.8599	C6—H6	0.9300
C1—C2	1.395 (3)	C7—H7	0.9301
C2—C3	1.376 (3)	C8—H8	0.9298
C3—C4	1.450 (3)	C9—H9	0.9301
C4—C5	1.492 (3)	C10—H10	0.9300
O1...N3 ⁱ	2.880 (3)	C5...H7 ^{vii}	3.0490
O1...C2 ⁱ	3.373 (3)	C6...H3B	2.5122
O1...N1 ⁱⁱ	2.818 (2)	C9...H6 ^{viii}	3.0512
O1...H2 ⁱ	2.6629	C9...H3B ^{ix}	2.8900
O1...H3A ⁱ	2.0609	H1...O1 ⁱⁱ	1.9577
O1...H1 ⁱⁱ	1.9577	H1...C1 ⁱⁱ	2.8745
O1...H10 ⁱⁱⁱ	2.8978	H1...H1 ⁱⁱ	2.5541
N1...O1 ⁱⁱ	2.818 (2)	H1...H2 ^{iv}	2.5843
N2...C2 ^{iv}	3.381 (3)	H2...H3A	2.4070
N3...C6	3.097 (3)	H2...O1 ^{vi}	2.6629
N3...C1 ^v	3.437 (3)	H2...H1 ⁱⁱⁱ	2.5843
N3...O1 ^{vi}	2.880 (3)	H3A...H2	2.4070
N2...H7 ^{vii}	2.7396	H3A...O1 ^{vi}	2.0609
N2...H10	2.7084	H3A...C1 ^{vi}	2.9723
N3...H6	2.7500	H3B...C5	2.6246
C1...N3 ^v	3.437 (3)	H3B...C6	2.5122
C2...N2 ⁱⁱⁱ	3.381 (3)	H3B...H6	2.2187
C2...C3 ^v	3.451 (3)	H3B...C9 ^x	2.8900
C2...C4 ^v	3.551 (3)	H3B...H9 ^x	2.5908
C2...O1 ^{vi}	3.373 (3)	H6...N3	2.7500
C3...C2 ^v	3.451 (3)	H6...C3	3.0017
C3...C3 ^v	3.460 (3)	H6...H3B	2.2187
C4...C2 ^v	3.551 (3)	H6...C9 ^{xi}	3.0512
C6...N3	3.097 (3)	H7...N2 ^{xii}	2.7396
C1...H1 ⁱⁱ	2.8745	H7...C4 ^{xii}	3.0979
C1...H10 ⁱⁱⁱ	2.7808	H7...C5 ^{xii}	3.0490

C1...H3A ⁱ	2.9723	H9...H3B ^{ix}	2.5908
C3...H6	3.0017	H10...N2	2.7084
C4...H7 ^{vii}	3.0979	H10...O1 ^{iv}	2.8978
C5...H3B	2.6246	H10...C1 ^{iv}	2.7808
N2—N1—C1	125.86 (15)	C4—C5—C10	119.25 (17)
N1—N2—C4	118.06 (15)	C5—C6—C7	119.8 (2)
N2—N1—H1	117.07	C6—C7—C8	120.6 (2)
C1—N1—H1	117.08	C7—C8—C9	120.0 (3)
C3—N3—H3A	119.99	C8—C9—C10	120.3 (3)
H3A—N3—H3B	120.00	C5—C10—C9	120.5 (2)
C3—N3—H3B	120.00	C1—C2—H2	119.41
O1—C1—C2	126.04 (17)	C3—C2—H2	119.42
N1—C1—C2	115.88 (16)	C5—C6—H6	120.10
O1—C1—N1	118.07 (16)	C7—C6—H6	120.11
C1—C2—C3	121.17 (17)	C6—C7—H7	119.73
N3—C3—C2	122.12 (17)	C8—C7—H7	119.67
N3—C3—C4	120.82 (16)	C7—C8—H8	120.00
C2—C3—C4	117.03 (16)	C9—C8—H8	119.96
C3—C4—C5	123.32 (16)	C8—C9—H9	119.85
N2—C4—C5	114.71 (16)	C10—C9—H9	119.87
N2—C4—C3	121.97 (16)	C5—C10—H10	119.76
C4—C5—C6	121.89 (18)	C9—C10—H10	119.74
C6—C5—C10	118.78 (18)		
C1—N1—N2—C4	-1.3 (3)	C3—C4—C5—C10	132.03 (19)
N2—N1—C1—O1	-178.29 (16)	N2—C4—C5—C6	129.2 (2)
N2—N1—C1—C2	1.9 (3)	N2—C4—C5—C10	-47.5 (2)
N1—N2—C4—C3	-0.7 (2)	C3—C4—C5—C6	-51.3 (3)
N1—N2—C4—C5	178.87 (15)	C4—C5—C6—C7	-176.1 (2)
O1—C1—C2—C3	179.65 (19)	C10—C5—C6—C7	0.6 (3)
N1—C1—C2—C3	-0.6 (3)	C4—C5—C10—C9	176.60 (19)
C1—C2—C3—N3	-179.27 (18)	C6—C5—C10—C9	-0.2 (3)
C1—C2—C3—C4	-1.1 (3)	C5—C6—C7—C8	-1.1 (4)
N3—C3—C4—N2	180.00 (1)	C6—C7—C8—C9	1.0 (4)
C2—C3—C4—C5	-177.67 (17)	C7—C8—C9—C10	-0.6 (4)
N3—C3—C4—C5	0.5 (3)	C8—C9—C10—C5	0.1 (3)
C2—C3—C4—N2	1.8 (3)		

Symmetry codes: (i) $x-1/2, -y+1/2, -z$; (ii) $-x, -y, -z$; (iii) $-x+1/2, y+1/2, z$; (iv) $-x+1/2, y-1/2, z$; (v) $-x+1, -y, -z$; (vi) $x+1/2, -y+1/2, -z$; (vii) $x-1/2, y, -z-1/2$; (viii) $-x+1, y-1/2, -z-1/2$; (ix) $-x+3/2, y-1/2, z$; (x) $-x+3/2, y+1/2, z$; (xi) $-x+1, y+1/2, -z-1/2$; (xii) $x+1/2, y, -z-1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1...O1 ⁱⁱ	0.86	1.96	2.818 (2)	180
N3—H3A...O1 ^{vi}	0.86	2.06	2.880 (3)	159

Symmetry codes: (ii) $-x, -y, -z$; (vi) $x+1/2, -y+1/2, -z$.