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Phthalazin-1(2*H*)-one

Orhan Büyükgüngör,[a] Mustafa Odabaşoğlu,[b]* B. Narayana,[c] A. M. Vijesh[c] and H. S. Yathirajan[d]

[a]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey, [b]Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey, [c]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [d]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India
Correspondence e-mail: muodabas@omu.edu.tr

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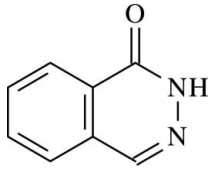
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.100; data-to-parameter ratio = 10.7.

The molecule of the title compound, $C_8H_6N_2O$, is almost planar, with a dihedral angle of 0.52 (7)° between the two rings. In the crystal structure, intermolecular N—H···O, C—H···N and C—H···O hydrogen bonds and π–π interactions link the molecules into a three-dimensional network. The π–π interaction occurs between the pyridazinone and benzene rings of the molecules at (x, y, z) and $(x-1, y, z)$; the centroid–centroid distance is 3.588 (1) Å and the plane–plane separation is 3.434 Å.

Related literature

For general background, see: Cheng *et al.* (1999). For bond-length data, see: Allen *et al.* (1987). For related literature, see: Etter (1990).



Experimental

Crystal data

$C_8H_6N_2O$
M_r = 146.15
Monoclinic, $P2_1/c$
a = 4.0321 (3) Å
b = 12.3412 (13) Å
c = 13.7513 (10) Å
β = 90.534 (6)°
V = 684.25 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.65 × 0.46 × 0.29 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED*; Stoe & Cie, 2002)
T_{min} = 0.944, T_{max} = 0.979
9171 measured reflections
1324 independent reflections
1064 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.100
S = 1.06
1324 reflections
124 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.92 (2)	1.92 (2)	2.8423 (16)	175.5 (17)
C5—H5···N2^{ii}	0.96 (2)	2.65 (2)	3.568 (2)	160.0 (15)
C6—H6···O1^{iii}	0.942 (17)	2.841 (17)	3.4298 (19)	121.6 (12)
C6—H6···O1^{iv}	0.942 (17)	2.835 (17)	3.664 (2)	147.5 (13)

Symmetry codes: (i) $-x+2, -y, -z+2$; (ii) $x-1, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2270).

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supplementary materials

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Phthalazin-1(2*H*)-one

O. Büyükgüngör, M. Odabasoglu, B. Narayana, A. M. Vijesh and H. S. Yathirajan

Comment

Phthalazines, also called benzo-orthodiazines or benzopyridazines, are a group of heterocyclic compounds isomeric with the cinnolines. The practical interest upon phthalazine derivatives is based on their widespread applications. Phthalazines, like other members of the isomeric diazine series, have found wide applications as therapeutic agents. Phthalazines are also commonly used as ligands in transition metal catalysis, as chemiluminescent materials and for optical applications (Cheng *et al.*, 1999). 2-Substituted-8-(4,6-dimethoxy- pyrimidin-2-yloxy)-4-methylphthalazin-1-one derivatives are used as herbicides. In view of the importance of the title compound, (I), we herein report its crystal structure.

In the molecule of the title compound, (I), (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The rings A (N1/N2/C1/C2/C7/C8) and B (C2—C7) are, of course, planar and they are also coplanar with a dihedral angle of A/B = 0.52 (7)°.

In the crystal structure, intermolecular N—H···O, C—H···N and C—H···O hydrogen bonds (Table 1) link the molecules, in which N—H···O bonds generate the centrosymmetric $R_2^2(8)$ dimers (Etter, 1990), and they are connected by C—H···O and C—H···N bonds to generate the edge-fussed [$R_3^2(8)$ $R_3^3(14)$] ring motifs (Fig. 2). In addition, the three-dimensional network including these motifs are also linked by π···π interactions, occurring between the *Cg*1—*Cg*2 rings (*Cg*1 and *Cg*2 are the centroids of rings A and B) of the molecules at (*x*, *y*, *z*) and (*x* − 1, *y*, *z*), with a centroid-to-centroid distance of 3.588 (1) Å and a plane-to-plane separation of 3.434 Å.

Experimental

A pure sample of the compound was obtained from Strides Arco Labs, Mangalore, India and crystallized from DMF (m.p. 528–530 K).

Refinement

H atoms were located in difference syntheses and refined isotropically [N—H = 0.92 (2) Å, U_{iso}(H) = 0.078 (6) Å^2; C—H = 0.942 (17)–0.975 (18) Å, U_{iso}(H) = 0.063 (5)–0.079 (5) Å^2].

Figures

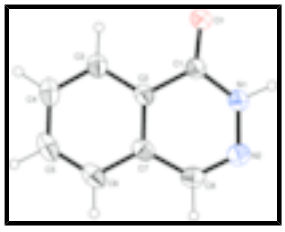


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

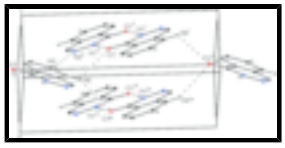


Fig. 2. A partial packing diagram for (I). H atoms not involved in hydrogen bonding have been omitted for clarity. Hydrogen bonds are shown as dashed lines [symmetry codes: (i) $x - 1/2, y + 1/2, 3/2 - z$; (ii) $x - 1, 1/2 - y, z - 1/2$; (iii) $x, 1/2 - y, z - 1/2$; (iv) $x + 1/2, y + 1/2, 3/2 - z$; (v) $x, y + 1, z$].

Phthalazin-1(2*H*)-one

Crystal data

$C_8H_6N_2O$	F_{000} = 304
M_r = 146.15	D_x = 1.419 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9171 reflections
a = 4.0321 (3) Å	θ = 3.0–27.9º
b = 12.3412 (13) Å	μ = 0.10 mm^{-1}
c = 13.7513 (10) Å	T = 296 K
β = 90.534 (6)º	Prism, colorless
V = 684.25 (10) Å^3	0.65 × 0.46 × 0.29 mm
Z = 4	

Data collection

Stoe IPDS II diffractometer	1324 independent reflections
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	1064 reflections with $I > 2\sigma(I)$
Monochromator: plane graphite	R_{int} = 0.044
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 26.0º
T = 296 K	θ_{min} = 3.0º
ω scans	h = −4→4
Absorption correction: integration (X-RED; Stoe & Cie, 2002)	k = −15→15
T_{min} = 0.944, T_{max} = 0.979	l = −16→16
9171 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	All H-atom parameters refined
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.0889P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
1324 reflections	$\Delta\rho_{max} = 0.12$ e Å^{-3}
124 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8204 (4)	0.04381 (11)	0.86523 (10)	0.0480 (4)
C2	0.7038 (3)	0.08027 (11)	0.77005 (9)	0.0440 (3)
C3	0.5213 (4)	0.01188 (13)	0.70937 (11)	0.0523 (4)
C4	0.4186 (4)	0.04883 (16)	0.62008 (12)	0.0623 (4)
C5	0.4969 (5)	0.15293 (16)	0.58975 (12)	0.0672 (5)
C6	0.6760 (4)	0.22069 (15)	0.64822 (12)	0.0607 (4)
C7	0.7822 (4)	0.18524 (12)	0.74036 (10)	0.0482 (4)
C8	0.9696 (4)	0.25138 (12)	0.80633 (12)	0.0560 (4)
N1	0.9897 (3)	0.11846 (10)	0.91799 (9)	0.0539 (3)
N2	1.0698 (3)	0.22166 (10)	0.89115 (10)	0.0586 (4)
O1	0.7743 (3)	−0.04865 (8)	0.89695 (8)	0.0663 (4)
H1	1.074 (5)	0.0989 (15)	0.9782 (15)	0.078 (6)*
H3	0.470 (4)	−0.0610 (15)	0.7317 (13)	0.063 (5)*
H4	0.291 (5)	0.0011 (15)	0.5808 (14)	0.076 (5)*
H5	0.421 (5)	0.1757 (15)	0.5269 (15)	0.079 (5)*
H6	0.728 (4)	0.2924 (14)	0.6304 (12)	0.069 (5)*
H8	1.030 (4)	0.3249 (15)	0.7875 (12)	0.063 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0569 (8)	0.0442 (7)	0.0428 (7)	0.0024 (6)	−0.0040 (6)	0.0005 (6)

C2	0.0469 (7)	0.0472 (7)	0.0380 (7)	0.0089 (6)	0.0003 (5)	0.0005 (5)
C3	0.0547 (9)	0.0567 (9)	0.0455 (8)	0.0057 (7)	−0.0029 (6)	−0.0031 (7)
C4	0.0610 (10)	0.0817 (12)	0.0439 (8)	0.0118 (8)	−0.0075 (7)	−0.0084 (8)
C5	0.0710 (11)	0.0895 (13)	0.0410 (8)	0.0258 (9)	−0.0023 (7)	0.0093 (8)
C6	0.0689 (10)	0.0630 (10)	0.0503 (9)	0.0176 (8)	0.0050 (7)	0.0148 (7)
C7	0.0502 (8)	0.0481 (8)	0.0463 (7)	0.0115 (6)	0.0055 (6)	0.0046 (6)
C8	0.0619 (9)	0.0430 (8)	0.0632 (9)	0.0020 (7)	0.0020 (7)	0.0045 (7)
N1	0.0704 (9)	0.0481 (7)	0.0430 (7)	−0.0025 (6)	−0.0099 (6)	0.0015 (5)
N2	0.0683 (9)	0.0470 (7)	0.0604 (8)	−0.0025 (6)	−0.0067 (6)	−0.0017 (6)
O1	0.0955 (9)	0.0494 (6)	0.0536 (6)	−0.0116 (6)	−0.0212 (6)	0.0114 (5)

Geometric parameters (Å, °)

C1—O1	1.2363 (17)	C5—C6	1.363 (3)
C1—N1	1.3533 (18)	C5—H5	0.96 (2)
C1—C2	1.4580 (18)	C6—C7	1.404 (2)
C2—C3	1.392 (2)	C6—H6	0.942 (17)
C2—C7	1.395 (2)	C7—C8	1.431 (2)
C3—C4	1.370 (2)	C8—N2	1.284 (2)
C3—H3	0.973 (18)	C8—H8	0.975 (18)
C4—C5	1.388 (3)	N1—N2	1.3656 (18)
C4—H4	0.947 (19)	N1—H1	0.92 (2)
O1—C1—N1	121.06 (13)	C4—C5—H5	118.1 (12)
O1—C1—C2	123.59 (13)	C5—C6—C7	119.80 (16)
N1—C1—C2	115.34 (12)	C5—C6—H6	122.7 (11)
C3—C2—C7	120.49 (13)	C7—C6—H6	117.5 (11)
C3—C2—C1	121.01 (13)	C2—C7—C6	119.04 (15)
C7—C2—C1	118.50 (13)	C2—C7—C8	117.64 (13)
C4—C3—C2	119.27 (15)	C6—C7—C8	123.32 (15)
C4—C3—H3	121.8 (10)	N2—C8—C7	124.93 (14)
C2—C3—H3	118.9 (10)	N2—C8—H8	115.4 (10)
C3—C4—C5	120.64 (16)	C7—C8—H8	119.7 (10)
C3—C4—H4	117.5 (12)	C1—N1—N2	127.55 (13)
C5—C4—H4	121.8 (11)	C1—N1—H1	118.8 (12)
C6—C5—C4	120.76 (15)	N2—N1—H1	113.6 (12)
C6—C5—H5	121.1 (12)	C8—N2—N1	116.01 (13)
O1—C1—C2—C3	1.9 (2)	C3—C2—C7—C8	179.84 (14)
N1—C1—C2—C3	−178.83 (14)	C1—C2—C7—C8	−0.86 (19)
O1—C1—C2—C7	−177.44 (14)	C5—C6—C7—C2	0.5 (2)
N1—C1—C2—C7	1.88 (19)	C5—C6—C7—C8	−179.68 (15)
C7—C2—C3—C4	−0.2 (2)	C2—C7—C8—N2	−0.4 (2)
C1—C2—C3—C4	−179.43 (13)	C6—C7—C8—N2	179.79 (15)
C2—C3—C4—C5	0.5 (2)	O1—C1—N1—N2	177.40 (15)
C3—C4—C5—C6	−0.3 (3)	C2—C1—N1—N2	−1.9 (2)
C4—C5—C6—C7	−0.2 (2)	C7—C8—N2—N1	0.5 (2)
C3—C2—C7—C6	−0.3 (2)	C1—N1—N2—C8	0.8 (2)
C1—C2—C7—C6	178.96 (13)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.92 (2)	1.92 (2)	2.8423 (16)	175.5 (17)
C5—H5···N2^{ii}	0.96 (2)	2.65 (2)	3.568 (2)	160.0 (15)
C6—H6···O1^{iii}	0.942 (17)	2.841 (17)	3.4298 (19)	121.6 (12)
C6—H6···O1^{iv}	0.942 (17)	2.835 (17)	3.664 (2)	147.5 (13)

Symmetry codes: (i) −*x*+2, −*y*, −*z*+2; (ii) *x*−1, −*y*+1/2, *z*−1/2; (iii) −*x*+1, *y*+1/2, −*z*+3/2; (iv) −*x*+2, *y*+1/2, −*z*+3/2.

Fig. 1

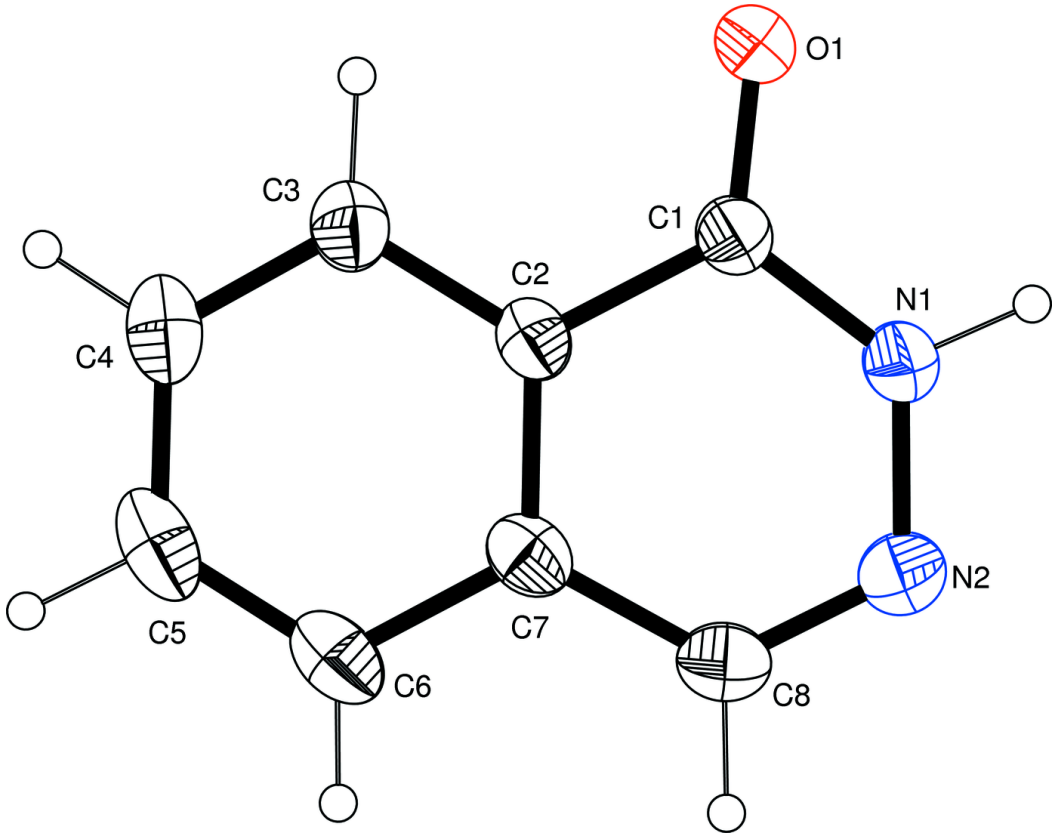
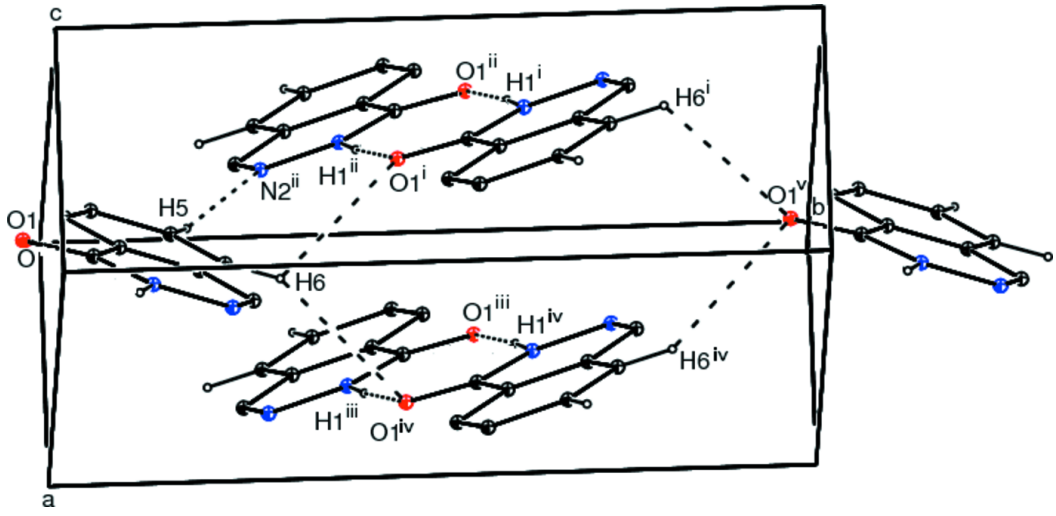


Fig. 2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a
b
O1
O
H5
H6
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H1ii
O1i
O1ii
H1i
H6i
O1v
O1iii
H1iv
H6iv
H1iii
O1iv