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Benzaldehyde propionylhydrazone

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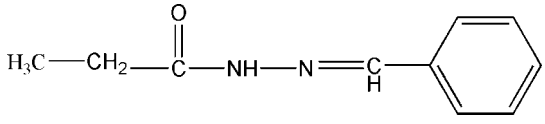
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.052; wR factor = 0.165; data-to-parameter ratio = 14.4.

The title compound, $C_{10}H_{12}N_2O$, was prepared by the reaction between benzaldehyde and propionylhydrazine. The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Allen *et al.* (1987); Sutherland & Hoy (1968); Tucker *et al.* (1975).



Experimental

Crystal data

$C_{10}H_{12}N_2O$
M_r = 176.22
Triclinic, $P\overline{1}$
a = 5.210 (3) Å
b = 8.838 (5) Å
c = 11.530 (6) Å
α = 111.419 (9)°
β = 91.916 (9)°
γ = 91.139 (9)°
V = 493.7 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.22 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
2478 measured reflections
1715 independent reflections
882 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.165
S = 1.02
1715 reflections
119 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1^{i}	0.86	2.07	2.906 (3)	163

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2367).

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supplementary materials

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Comment

As an extension of our work on the structural characterization of Schiff base compounds, we here report the structure of the title molecule (I). The title compound (I), is nearly planar. In (I) (Fig. 1), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The C7—N1 distance of 1.273 (3) Å is similar to the distance of 1.287 Å reported by Tucker *et al.* (1975). The C8—O1 distance of 1.228 (3) Å is shorter than the reported distance of 1.298 Å by Sutherland & Hoy (1968).

The crystal structure of (I) is stabilized by intermolecular N—H···O hydrogen bonds (Table 1).

Experimental

A mixture of the benzaldehyde (0.1 mol), and propionylhydrazine (0.1 mol) was stirred in refluxing ethanol (30 ml) for 5 h to afford the title compound (I) (0.087 mol, yield 87%). Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

H atoms were located geometrically and allowed to ride on their attached atoms, with C—H = 0.93–0.97 Å, N—H = 0.86 Å and with U_{iso}(H) = 1.2–1.5U_{eq}(C, N).

Figures

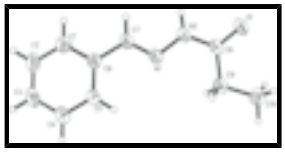

Fig. 1. The structure of the title compound (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Benzaldehyde propionylhydrazone

Crystal data

$C_{10}H_{12}N_2O$	V = 493.7 (5) Å^3
M_r = 176.22	Z = 2
Triclinic, $P\overline{1}$	F_{000} = 188
Hall symbol: -P 1	D_x = 1.185 Mg m^{-3}
a = 5.210 (3) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
b = 8.838 (5) Å	θ = 1.9–25.0º
c = 11.530 (6) Å	μ = 0.08 mm^{-1}

α = 111.419 (9)º	T = 293 (2) K
β = 91.916 (9)º	Block, colourless
γ = 91.139 (9)º	0.22 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer	882 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.020
Monochromator: graphite	θ_{max} = 25.0º
T = 293(2) K	θ_{min} = 1.9º
φ and ω scans	h = −6→6
Absorption correction: none	k = −10→10
2478 measured reflections	l = −13→10
1715 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.052	H-atom parameters constrained
$wR(F^2)$ = 0.165	$w = 1/[\sigma^2(F_o^2) + (0.0829P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
1715 reflections	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
119 parameters	$\Delta\rho_{min}$ = −0.18 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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	−0.4450 (3)	−0.0595 (2)	0.33336 (16)	0.0687 (6)
N1	−0.0417 (4)	0.2515 (2)	0.5372 (2)	0.0556 (6)
N2	−0.2421 (4)	0.1394 (2)	0.49157 (19)	0.0597 (6)

H2	−0.3550	0.1312	0.5419	0.072*
C1	0.1970 (6)	0.5178 (4)	0.8455 (3)	0.0775 (9)
H1	0.0842	0.4834	0.8924	0.093*
C2	0.3860 (7)	0.6354 (4)	0.9060 (3)	0.0863 (10)
H2A	0.3992	0.6788	0.9927	0.104*
C3	0.5519 (6)	0.6874 (4)	0.8390 (3)	0.0784 (10)
H3	0.6796	0.7657	0.8795	0.094*
C4	0.5301 (6)	0.6234 (4)	0.7106 (3)	0.0813 (10)
H4	0.6419	0.6596	0.6643	0.098*
C5	0.3428 (5)	0.5058 (3)	0.6507 (3)	0.0682 (9)
H5	0.3307	0.4626	0.5640	0.082*
C6	0.1727 (5)	0.4508 (3)	0.7172 (2)	0.0535 (7)
C7	−0.0300 (5)	0.3266 (3)	0.6549 (3)	0.0596 (7)
H7	−0.1529	0.3024	0.7027	0.071*
C8	−0.2668 (5)	0.0419 (3)	0.3702 (3)	0.0536 (7)
C9	−0.0709 (5)	0.0639 (3)	0.2847 (2)	0.0641 (8)
H9A	0.0980	0.0440	0.3131	0.077*
H9B	−0.0703	0.1757	0.2893	0.077*
C10	−0.1205 (7)	−0.0485 (4)	0.1498 (3)	0.0891 (11)
H10A	−0.1256	−0.1594	0.1447	0.134*
H10B	0.0147	−0.0328	0.1003	0.134*
H10C	−0.2820	−0.0242	0.1191	0.134*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0640 (13)	0.0637 (12)	0.0708 (13)	−0.0252 (10)	−0.0097 (10)	0.0181 (10)
N1	0.0564 (14)	0.0497 (12)	0.0561 (14)	−0.0141 (10)	−0.0086 (11)	0.0157 (11)
N2	0.0586 (14)	0.0567 (13)	0.0576 (14)	−0.0214 (11)	−0.0017 (11)	0.0149 (12)
C1	0.096 (2)	0.076 (2)	0.0572 (19)	−0.0216 (18)	−0.0023 (17)	0.0216 (17)
C2	0.104 (3)	0.075 (2)	0.061 (2)	−0.018 (2)	−0.018 (2)	0.0056 (18)
C3	0.070 (2)	0.0627 (19)	0.084 (2)	−0.0173 (16)	−0.0155 (19)	0.0081 (19)
C4	0.077 (2)	0.074 (2)	0.078 (2)	−0.0273 (17)	−0.0031 (17)	0.0126 (18)
C5	0.0701 (19)	0.0655 (18)	0.0564 (17)	−0.0216 (15)	0.0000 (15)	0.0090 (15)
C6	0.0602 (17)	0.0448 (14)	0.0523 (16)	−0.0039 (13)	−0.0010 (14)	0.0147 (14)
C7	0.0617 (18)	0.0545 (16)	0.0608 (18)	−0.0142 (13)	−0.0019 (14)	0.0203 (15)
C8	0.0488 (16)	0.0488 (15)	0.0606 (18)	−0.0080 (13)	−0.0070 (14)	0.0183 (14)
C9	0.0638 (19)	0.0571 (16)	0.0630 (18)	−0.0106 (14)	−0.0018 (15)	0.0129 (15)
C10	0.117 (3)	0.078 (2)	0.063 (2)	−0.0226 (19)	0.0082 (18)	0.0168 (17)

Geometric parameters (Å, °)

O1—C8	1.228 (3)	C4—H4	0.9300
N1—C7	1.273 (3)	C5—C6	1.382 (4)
N1—N2	1.374 (3)	C5—H5	0.9300
N2—C8	1.349 (3)	C6—C7	1.471 (3)
N2—H2	0.8600	C7—H7	0.9300
C1—C6	1.378 (3)	C8—C9	1.500 (4)
C1—C2	1.386 (4)	C9—C10	1.519 (3)

C1—H1	0.9300	C9—H9A	0.9700
C2—C3	1.358 (4)	C9—H9B	0.9700
C2—H2A	0.9300	C10—H10A	0.9600
C3—C4	1.378 (4)	C10—H10B	0.9600
C3—H3	0.9300	C10—H10C	0.9600
C4—C5	1.378 (3)		
C7—N1—N2	115.5 (2)	C1—C6—C7	120.5 (3)
C8—N2—N1	121.9 (2)	C5—C6—C7	121.9 (2)
C8—N2—H2	119.0	N1—C7—C6	121.7 (3)
N1—N2—H2	119.0	N1—C7—H7	119.1
C6—C1—C2	121.4 (3)	C6—C7—H7	119.1
C6—C1—H1	119.3	O1—C8—N2	120.1 (2)
C2—C1—H1	119.3	O1—C8—C9	122.5 (2)
C3—C2—C1	120.1 (3)	N2—C8—C9	117.4 (2)
C3—C2—H2A	119.9	C8—C9—C10	113.1 (2)
C1—C2—H2A	119.9	C8—C9—H9A	109.0
C2—C3—C4	119.6 (3)	C10—C9—H9A	109.0
C2—C3—H3	120.2	C8—C9—H9B	109.0
C4—C3—H3	120.2	C10—C9—H9B	109.0
C5—C4—C3	120.1 (3)	H9A—C9—H9B	107.8
C5—C4—H4	120.0	C9—C10—H10A	109.5
C3—C4—H4	120.0	C9—C10—H10B	109.5
C4—C5—C6	121.2 (3)	H10A—C10—H10B	109.5
C4—C5—H5	119.4	C9—C10—H10C	109.5
C6—C5—H5	119.4	H10A—C10—H10C	109.5
C1—C6—C5	117.6 (3)	H10B—C10—H10C	109.5
C7—N1—N2—C8	−174.7 (2)	C4—C5—C6—C7	179.3 (3)
C6—C1—C2—C3	0.2 (5)	N2—N1—C7—C6	−179.6 (2)
C1—C2—C3—C4	0.5 (5)	C1—C6—C7—N1	−173.1 (3)
C2—C3—C4—C5	−0.8 (5)	C5—C6—C7—N1	7.6 (4)
C3—C4—C5—C6	0.6 (5)	N1—N2—C8—O1	178.2 (2)
C2—C1—C6—C5	−0.4 (4)	N1—N2—C8—C9	−2.0 (4)
C2—C1—C6—C7	−179.7 (3)	O1—C8—C9—C10	1.3 (4)
C4—C5—C6—C1	0.0 (4)	N2—C8—C9—C10	−178.4 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.86	2.07	2.906 (3)	163

Symmetry codes: (i) −*x*−1, −*y*, −*z*+1.

Fig. 1