Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-(1-Phenylethylidene)acetohydrazide

Huan-Mei Guo

Department of Chemistry, Weifang College, Weifang 261061, People's Republic of China
Correspondence e-mail: huanmeiguo@163.com

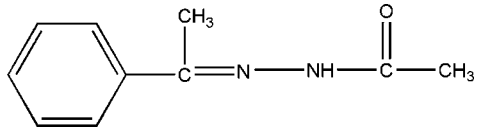
Received 30 May 2007; accepted 31 May 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.117; data-to-parameter ratio = 15.5.

The title compound, $C_{10}H_{12}N_2O$, was prepared by the reaction between hypnone and acetohydrazide. Molecules form centrosymmetric dimers through N—H···O and weak C—H···O hydrogen bonds. Weak interactions between the dimers and intramolecular C—H···N hydrogen-bond interactions stabilize the crystal packing.

Related literature

For related literature, see: Cimerman *et al.* (1997); Sutherland & Hoy (1968); Tucker *et al.* (1975).



Experimental

Crystal data

$C_{10}H_{12}N_2O$
M_r = 176.22
Monoclinic, $P2_1/c$
a = 5.3681 (18) Å
b = 9.361 (3) Å
c = 19.033 (6) Å
β = 95.496 (6)°
V = 952.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 (2) K
0.26 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
5285 measured reflections
1940 independent reflections
882 reflections with $I > 2\sigma(I)$
R_{int} = 0.070

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.117
S = 1.03
1940 reflections
125 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.91 (2)	2.11 (2)	3.011 (3)	172.2 (18)
C8—H8C···N2	0.96	2.44	2.827 (3)	103
C8—H8C···O1^{i}	0.96	2.35	3.273 (3)	160

Symmetry code: (i) $-x+3, -y+1, -z+1$.

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2312).

References

Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cimerman, Z., Galic, N. & Bosner, B. (1997). *Anal. Chim. Acta*, **343**, 145–153.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sutherland, H. H. & Hoy, T. G. (1968). *Acta Cryst.* B**24**, 1207–1213.
Tucker, P. A., Hoekstra, A., ten Cate, J. M. & Vos, A. (1975). *Acta Cryst.* B**31**, 733–737.

supplementary materials

Acta Cryst. (2007). E**63**, o3123 [**doi:10.1107/S1600536807026748**]

N'-(1-Phenylethylidene)acetohydrazide

H.-M. Guo

Comment

As part of our search for new schiff base compounds we synthesized the title compound (I), and we report its structure here.

The molecules are linked together to form two dimer by N21—H2A···O1^{i} and weak C—H···O^{i} hydrogen bonds [symmetry code: (i) − *x* + 3, − *y* + 1, − *z* + 1] (Table 2 and Fig. 2). The structure is stabilized by weak-interactions between the dimers and intarmolecular C8—H8C···N2 hydrogen bonding interactions.

Experimental

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

Refinement

The H atom bound to the N2 atom were found from a difference Fourier map and refined freely. The other H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H = 0.93–0.96 Å, and with U_{iso} = 1.2(C) or 1.5U_{eq}(C_{methyl}).

Figures

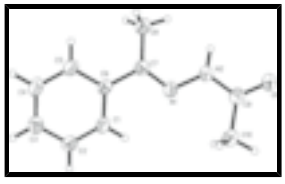


Fig. 1. View of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

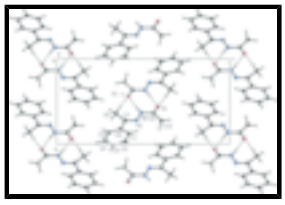


Fig. 2. A view of the N—H.·O and weak C—H.·O hydrogen-bonded dimer. [Symmetry code: (*a*) − *x* + 3, − *y* + 1, − *z* + 1].

N'-(1-Phenylethylidene)acetohydrazide

Crystal data

$C_{10}H_{12}N_2O$ $Z = 4$

M_r = 176.22	F_{000} = 376
Monoclinic, $P2_1/c$	D_x = 1.229 Mg m^{-3}
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 5.3681 (18) Å	θ = 2.2–26.3º
b = 9.361 (3) Å	μ = 0.08 mm^{-1}
c = 19.033 (6) Å	T = 294 (2) K
β = 95.496 (6)º	Block, colourless
V = 952.0 (5) Å^3	0.26 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer	882 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.070
Monochromator: graphite	θ_{max} = 26.3º
T = 294(2) K	θ_{min} = 2.2º
φ and ω scans	h = −6→6
Absorption correction: none	k = −9→11
5285 measured reflections	l = −23→19
1940 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
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.117	$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
1940 reflections	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
125 parameters	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
1 restraint	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.067 (6)

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 calculat-

ing *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	1.4564 (3)	0.56158 (18)	0.58573 (8)	0.0711 (6)
N1	1.0181 (3)	0.72134 (19)	0.46283 (10)	0.0492 (5)
N2	1.2145 (4)	0.6349 (2)	0.48995 (10)	0.0527 (6)
C1	0.5972 (4)	0.8765 (2)	0.41812 (12)	0.0505 (7)
H1	0.6218	0.8495	0.4653	0.061*
C2	0.4048 (5)	0.9687 (3)	0.39673 (12)	0.0586 (7)
H2	0.3014	1.0030	0.4294	0.070*
C3	0.3650 (5)	1.0105 (3)	0.32713 (14)	0.0616 (8)
H3	0.2363	1.0736	0.3128	0.074*
C4	0.5168 (5)	0.9580 (3)	0.27914 (13)	0.0611 (7)
H4	0.4898	0.9851	0.2320	0.073*
C5	0.7111 (4)	0.8644 (2)	0.30053 (12)	0.0560 (7)
H5	0.8125	0.8294	0.2675	0.067*
C6	0.7554 (4)	0.8228 (2)	0.37083 (11)	0.0431 (6)
C7	0.9639 (4)	0.7243 (2)	0.39541 (12)	0.0463 (6)
C8	1.0931 (5)	0.6416 (2)	0.34212 (12)	0.0623 (8)
H8A	1.2002	0.7043	0.3188	0.093*
H8B	0.9704	0.6006	0.3080	0.093*
H8C	1.1915	0.5668	0.3655	0.093*
C9	1.2788 (5)	0.6354 (3)	0.56074 (13)	0.0528 (7)
C10	1.1281 (5)	0.7261 (3)	0.60558 (12)	0.0659 (8)
H10A	1.1863	0.7125	0.6544	0.099*
H10B	0.9550	0.6994	0.5979	0.099*
H10C	1.1462	0.8248	0.5932	0.099*
H2A	1.302 (4)	0.576 (2)	0.4637 (10)	0.070 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0738 (13)	0.0854 (13)	0.0519 (11)	0.0266 (11)	−0.0058 (10)	0.0042 (9)
N1	0.0445 (12)	0.0578 (12)	0.0446 (12)	−0.0008 (10)	−0.0001 (10)	0.0073 (10)
N2	0.0549 (14)	0.0599 (14)	0.0423 (13)	0.0097 (12)	−0.0002 (11)	0.0043 (11)
C1	0.0533 (16)	0.0593 (15)	0.0381 (14)	−0.0005 (13)	0.0000 (12)	0.0051 (12)
C2	0.0571 (17)	0.0710 (18)	0.0472 (16)	0.0068 (15)	0.0029 (13)	−0.0075 (13)
C3	0.0572 (18)	0.0659 (18)	0.0598 (18)	0.0079 (14)	−0.0053 (15)	0.0019 (14)
C4	0.0628 (19)	0.0726 (18)	0.0464 (16)	−0.0014 (15)	−0.0031 (15)	0.0140 (14)
C5	0.0569 (17)	0.0689 (17)	0.0421 (15)	−0.0012 (14)	0.0039 (12)	0.0026 (13)
C6	0.0434 (14)	0.0492 (15)	0.0362 (13)	−0.0071 (12)	0.0011 (11)	0.0000 (11)
C7	0.0466 (15)	0.0484 (14)	0.0433 (14)	−0.0056 (12)	0.0016 (12)	−0.0015 (12)
C8	0.0690 (18)	0.0666 (16)	0.0499 (15)	0.0078 (14)	−0.0017 (13)	−0.0038 (13)
C9	0.0566 (17)	0.0555 (16)	0.0460 (16)	−0.0005 (14)	0.0032 (13)	0.0029 (13)
C10	0.0755 (19)	0.0724 (18)	0.0489 (15)	0.0095 (15)	0.0013 (14)	−0.0001 (13)

Geometric parameters (Å, °)

O1—C9	1.235 (3)	C4—H4	0.9300
N1—C7	1.289 (2)	C5—C6	1.392 (3)
N1—N2	1.389 (2)	C5—H5	0.9300
N2—C9	1.358 (3)	C6—C7	1.490 (3)
N2—H2A	0.904 (10)	C7—C8	1.498 (3)
C1—C2	1.378 (3)	C8—H8A	0.9600
C1—C6	1.389 (3)	C8—H8B	0.9600
C1—H1	0.9300	C8—H8C	0.9600
C2—C3	1.378 (3)	C9—C10	1.496 (3)
C2—H2	0.9300	C10—H10A	0.9600
C3—C4	1.372 (3)	C10—H10B	0.9600
C3—H3	0.9300	C10—H10C	0.9600
C4—C5	1.393 (3)		
C7—N1—N2	118.3 (2)	C1—C6—C7	120.5 (2)
C9—N2—N1	118.6 (2)	C5—C6—C7	121.9 (2)
C9—N2—H2A	117.1 (14)	N1—C7—C6	114.7 (2)
N1—N2—H2A	124.3 (14)	N1—C7—C8	126.0 (2)
C2—C1—C6	121.5 (2)	C6—C7—C8	119.32 (19)
C2—C1—H1	119.2	C7—C8—H8A	109.5
C6—C1—H1	119.2	C7—C8—H8B	109.5
C1—C2—C3	120.3 (2)	H8A—C8—H8B	109.5
C1—C2—H2	119.8	C7—C8—H8C	109.5
C3—C2—H2	119.8	H8A—C8—H8C	109.5
C4—C3—C2	119.4 (2)	H8B—C8—H8C	109.5
C4—C3—H3	120.3	O1—C9—N2	119.6 (2)
C2—C3—H3	120.3	O1—C9—C10	122.5 (2)
C3—C4—C5	120.4 (2)	N2—C9—C10	117.9 (2)
C3—C4—H4	119.8	C9—C10—H10A	109.5
C5—C4—H4	119.8	C9—C10—H10B	109.5
C6—C5—C4	120.8 (2)	H10A—C10—H10B	109.5
C6—C5—H5	119.6	C9—C10—H10C	109.5
C4—C5—H5	119.6	H10A—C10—H10C	109.5
C1—C6—C5	117.6 (2)	H10B—C10—H10C	109.5
C7—N1—N2—C9	177.5 (2)	N2—N1—C7—C6	−178.45 (18)
C6—C1—C2—C3	−0.1 (3)	N2—N1—C7—C8	0.4 (3)
C1—C2—C3—C4	0.7 (3)	C1—C6—C7—N1	−15.2 (3)
C2—C3—C4—C5	−0.6 (4)	C5—C6—C7—N1	164.71 (19)
C3—C4—C5—C6	−0.2 (3)	C1—C6—C7—C8	165.8 (2)
C2—C1—C6—C5	−0.6 (3)	C5—C6—C7—C8	−14.2 (3)
C2—C1—C6—C7	179.33 (19)	N1—N2—C9—O1	−178.5 (2)
C4—C5—C6—C1	0.8 (3)	N1—N2—C9—C10	1.9 (3)
C4—C5—C6—C7	−179.2 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N2—H2A···O1^{i}	0.91 (2)	2.11 (2)	3.011 (3)	172.2 (18)
C8—H8C···N2	0.96	2.44	2.827 (3)	103
C8—H8C···O1^{i}	0.96	2.35	3.273 (3)	160

Symmetry codes: (i) −*x*+3, −*y*+1, −*z*+1.

Fig. 1

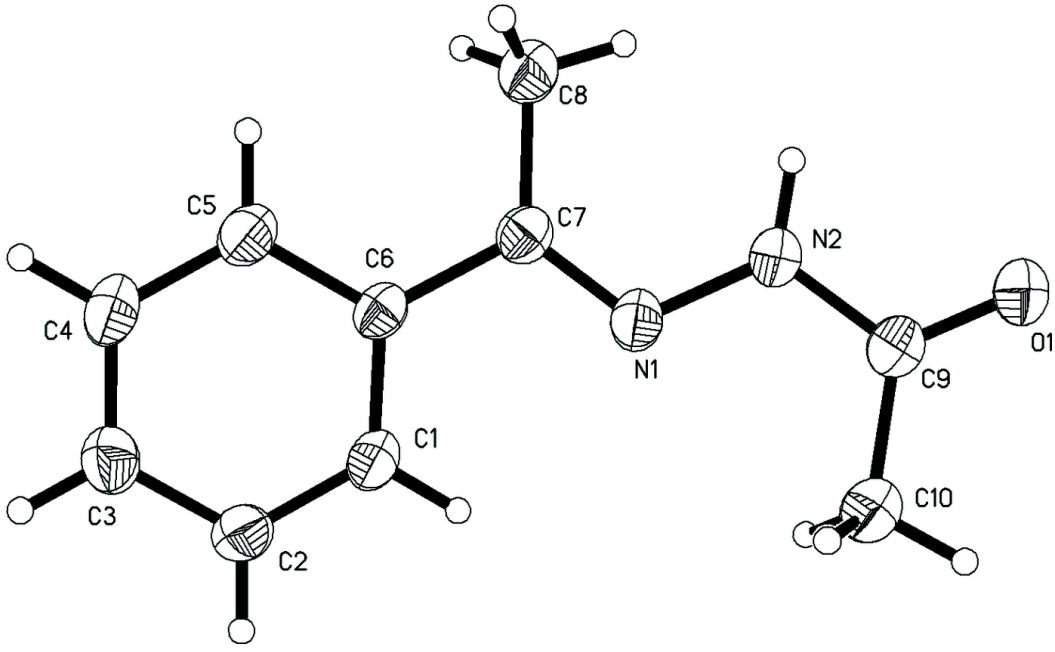


Fig. 2