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N′-[1-(2-Hydroxyphenyl)ethylidene]-acetohydrazide

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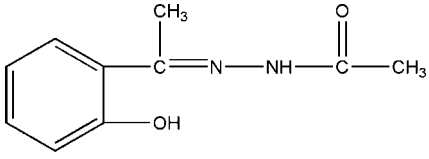
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.127; data-to-parameter ratio = 14.6.

The title compound, $C_{10}H_{12}N_2O_2$, was prepared by the reaction of *o*-hydroxyhypnone and acetohydrazide. In the structure, there are intramolecular C—H···N and O—H···N, and intermolecular N—H···O and C—H···O hydrogen-bond interactions.

Related literature

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



Experimental

Crystal data

$C_{10}H_{12}N_2O_2$
M_r = 192.22
Monoclinic, $P2_1/c$
a = 7.547 (2) Å
b = 13.586 (4) Å
c = 9.642 (3) Å
β = 103.427 (5)°
V = 961.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.20 × 0.18 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
5410 measured reflections
1954 independent reflections
1423 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.127
S = 1.02
1954 reflections
134 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.81	2.5239 (18)	145
N2—H2A···O2^{i}	0.894 (10)	2.019 (11)	2.8951 (19)	166.5 (17)
C11—H11C···N2	0.96	2.45	2.845 (2)	104
C11—H11C···O2^{i}	0.96	2.57	3.406 (2)	146

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

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: AT2311).

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.

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supplementary materials

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N'-[1-(2-Hydroxyphenyl)ethylidene]acetohydrazide

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Comment

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

All of the bond lengths and angles in (I) (Fig. 1) are in normal ranges. The molecular and crystal structure is stabilized by the intramolecular C—H···N and O—H···N, and intermolecular N—H···O and C—H···O hydrogen bonding interactions.

Experimental

A mixture of the *o*-hydroxyhypnone (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 was found from a difference Fourier map and refined freely. The remained H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H = 0.93 − 0.96Å and O—H = 0.82Å and with U_{iso}=1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}, $O_{hydroxyl}$).

Figures

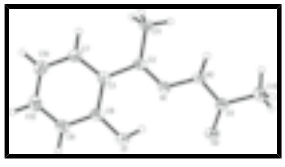

Fig. 1. The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

N'-[1-(2-Hydroxyphenyl)ethylidene]acetohydrazide

Crystal data

$C_{10}H_{12}N_2O_2$	Z = 4
M_r = 192.22	F_{000} = 408
Monoclinic, $P2_1/c$	D_x = 1.328 Mg m^{-3}
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.547 (2) Å	θ = 2.6–26.4º
b = 13.586 (4) Å	μ = 0.09 mm^{-1}
c = 9.642 (3) Å	T = 294 (2) K
β = 103.427 (5)º	Block, colourless

V = 961.7 (5) Å^3	0.20 × 0.18 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer	1423 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.029
Monochromator: graphite	θ_{max} = 26.4º
T = 294(2) K	θ_{min} = 2.6º
φ and ω scans	h = −9→9
Absorption correction: none	k = −10→16
5410 measured reflections	l = −12→11
1954 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
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.127	$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 0.1565P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
1954 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
134 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
N1	0.67833 (17)	0.88541 (10)	0.06106 (13)	0.0357 (3)
C2	0.7178 (2)	0.96368 (11)	−0.00015 (15)	0.0327 (4)
C3	0.8130 (2)	1.04027 (11)	0.09679 (15)	0.0337 (4)

N2	0.59270 (18)	0.80749 (10)	−0.01543 (13)	0.0375 (3)
C5	0.5327 (2)	0.73504 (12)	0.05823 (16)	0.0383 (4)
O2	0.54386 (18)	0.74213 (9)	0.18607 (12)	0.0526 (4)
C7	0.8664 (2)	1.12830 (12)	0.04435 (18)	0.0433 (4)
H7	0.8404	1.1384	−0.0537	0.052*
C8	0.8558 (2)	1.02813 (12)	0.24634 (16)	0.0377 (4)
C9	0.9474 (2)	1.10172 (13)	0.33407 (18)	0.0463 (4)
H9	0.9761	1.0928	0.4324	0.056*
C10	0.9563 (3)	1.20063 (13)	0.1329 (2)	0.0501 (5)
H10	0.9902	1.2586	0.0948	0.060*
C11	0.6710 (2)	0.97978 (13)	−0.15799 (16)	0.0434 (4)
H11A	0.7795	0.9752	−0.1935	0.065*
H11B	0.6180	1.0439	−0.1787	0.065*
H11C	0.5854	0.9306	−0.2030	0.065*
C12	0.9960 (2)	1.18695 (13)	0.27825 (19)	0.0489 (5)
H12	1.0562	1.2360	0.3385	0.059*
C13	0.4561 (3)	0.64741 (13)	−0.0270 (2)	0.0539 (5)
H13A	0.5521	0.6014	−0.0287	0.081*
H13B	0.4001	0.6674	−0.1227	0.081*
H13C	0.3666	0.6169	0.0152	0.081*
O1	0.81218 (19)	0.94621 (9)	0.31076 (11)	0.0531 (4)
H1	0.7625	0.9065	0.2500	0.080*
H2A	0.575 (2)	0.8027 (14)	−0.1101 (10)	0.054 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0430 (8)	0.0360 (7)	0.0278 (6)	0.0011 (6)	0.0075 (5)	−0.0009 (5)
C2	0.0331 (8)	0.0379 (8)	0.0283 (7)	0.0082 (6)	0.0094 (6)	0.0022 (6)
C3	0.0342 (8)	0.0353 (8)	0.0324 (8)	0.0053 (6)	0.0096 (6)	0.0020 (6)
N2	0.0516 (8)	0.0379 (8)	0.0232 (6)	−0.0013 (6)	0.0089 (6)	−0.0016 (6)
C5	0.0454 (9)	0.0389 (9)	0.0320 (8)	0.0040 (7)	0.0119 (7)	0.0026 (7)
O2	0.0809 (9)	0.0502 (8)	0.0298 (6)	−0.0026 (6)	0.0192 (6)	0.0023 (5)
C7	0.0511 (10)	0.0420 (9)	0.0381 (8)	0.0014 (8)	0.0129 (7)	0.0057 (7)
C8	0.0411 (9)	0.0405 (9)	0.0323 (8)	0.0021 (7)	0.0101 (6)	0.0006 (7)
C9	0.0525 (10)	0.0519 (11)	0.0345 (8)	−0.0021 (8)	0.0100 (7)	−0.0070 (8)
C10	0.0576 (11)	0.0389 (9)	0.0560 (11)	−0.0049 (8)	0.0175 (9)	0.0026 (8)
C11	0.0547 (10)	0.0455 (9)	0.0294 (8)	0.0031 (8)	0.0085 (7)	0.0049 (7)
C12	0.0481 (10)	0.0463 (10)	0.0530 (10)	−0.0057 (8)	0.0129 (8)	−0.0131 (8)
C13	0.0718 (13)	0.0455 (10)	0.0475 (10)	−0.0097 (9)	0.0197 (9)	−0.0059 (8)
O1	0.0782 (9)	0.0507 (8)	0.0273 (6)	−0.0141 (6)	0.0060 (6)	0.0036 (5)

Geometric parameters (Å, °)

N1—C2	1.284 (2)	C8—C9	1.386 (2)
N1—N2	1.3641 (18)	C9—C12	1.363 (2)
C2—C3	1.470 (2)	C9—H9	0.9300
C2—C11	1.496 (2)	C10—C12	1.376 (3)
C3—C7	1.394 (2)	C10—H10	0.9300

C3—C8	1.412 (2)	C11—H11A	0.9600
N2—C5	1.3520 (19)	C11—H11B	0.9600
N2—H2A	0.894 (9)	C11—H11C	0.9600
C5—O2	1.2197 (19)	C12—H12	0.9300
C5—C13	1.486 (2)	C13—H13A	0.9600
C7—C10	1.373 (2)	C13—H13B	0.9600
C7—H7	0.9300	C13—H13C	0.9600
C8—O1	1.3520 (19)	O1—H1	0.8200
C2—N1—N2	121.70 (12)	C8—C9—H9	119.5
N1—C2—C3	115.17 (13)	C7—C10—C12	119.73 (16)
N1—C2—C11	124.28 (14)	C7—C10—H10	120.1
C3—C2—C11	120.55 (14)	C12—C10—H10	120.1
C7—C3—C8	116.98 (15)	C2—C11—H11A	109.5
C7—C3—C2	121.10 (14)	C2—C11—H11B	109.5
C8—C3—C2	121.92 (14)	H11A—C11—H11B	109.5
C5—N2—N1	117.09 (12)	C2—C11—H11C	109.5
C5—N2—H2A	119.6 (12)	H11A—C11—H11C	109.5
N1—N2—H2A	123.3 (12)	H11B—C11—H11C	109.5
O2—C5—N2	121.36 (15)	C9—C12—C10	120.14 (17)
O2—C5—C13	123.33 (15)	C9—C12—H12	119.9
N2—C5—C13	115.31 (13)	C10—C12—H12	119.9
C10—C7—C3	122.09 (15)	C5—C13—H13A	109.5
C10—C7—H7	119.0	C5—C13—H13B	109.5
C3—C7—H7	119.0	H13A—C13—H13B	109.5
O1—C8—C9	116.97 (14)	C5—C13—H13C	109.5
O1—C8—C3	122.88 (14)	H13A—C13—H13C	109.5
C9—C8—C3	120.15 (15)	H13B—C13—H13C	109.5
C12—C9—C8	120.92 (16)	C8—O1—H1	109.5
C12—C9—H9	119.5		
N2—N1—C2—C3	−178.91 (13)	C2—C3—C7—C10	−179.66 (15)
N2—N1—C2—C11	1.9 (2)	C7—C3—C8—O1	−179.77 (15)
N1—C2—C3—C7	178.95 (14)	C2—C3—C8—O1	−0.3 (2)
C11—C2—C3—C7	−1.8 (2)	C7—C3—C8—C9	−0.2 (2)
N1—C2—C3—C8	−0.5 (2)	C2—C3—C8—C9	179.30 (14)
C11—C2—C3—C8	178.70 (14)	O1—C8—C9—C12	−179.73 (15)
C2—N1—N2—C5	−170.30 (13)	C3—C8—C9—C12	0.7 (3)
N1—N2—C5—O2	4.7 (2)	C3—C7—C10—C12	0.1 (3)
N1—N2—C5—C13	−174.46 (14)	C8—C9—C12—C10	−0.8 (3)
C8—C3—C7—C10	−0.2 (2)	C7—C10—C12—C9	0.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.81	2.5239 (18)	145
N2—H2A···O2^{i}	0.894 (10)	2.019 (11)	2.8951 (19)	166.5 (17)
C11—H11C···N2	0.96	2.45	2.845 (2)	104
C11—H11C···O2^{i}	0.96	2.57	3.406 (2)	146

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

Fig. 1