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(*E*)-*N*′-[1-(4-Aminophenyl)ethylidene]-benzohydrazide

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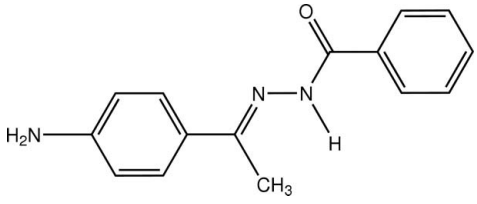
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.156; data-to-parameter ratio = 13.2.

Crystals of the title compound, $C_{15}H_{15}N_3O$, were obtained from a condensation reaction of benzohydrazide and 1-(4-aminophenyl)ethanone. The molecule assumes an *E* configuration with the aminophenyl and benzohydrazide units located on opposite sites of the C=N double bond. In the crystal structure, the benzene rings of the molecule are slightly twisted with respect to the central hydrazide, the dihedral angles being 18.22 (12) and 27.62 (12)°. The crystal structure contains intermolecular N—H···O and weak C—H···N hydrogen bonding.

Related literature

For general background, see: Okabe *et al.* (1993); Shan *et al.* (2003). For a related structure, see: Shan *et al.* (2008).



Experimental

Crystal data

$C_{15}H_{15}N_3O$ M_r = 253.30
Monoclinic, $P2_1/n$
a = 12.261 (9) Å
b = 5.324 (4) Å
c = 19.882 (15) Å
β = 94.57 (2)°
V = 1293.7 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.42 × 0.36 × 0.32 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: none
10914 measured reflections
2303 independent reflections
1594 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.156
S = 1.05
2303 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O1^{i}	0.86	2.44	3.169 (3)	143
C15—H15C···N2^{ii}	0.96	2.62	3.468 (3)	147

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); 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: XU2432).

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supplementary materials

Acta Cryst. (2008). E**64**, o1363 [**doi:10.1107/S1600536808019004**]

(*E*)-*N*'-[1-(4-Aminophenyl)ethylidene]benzohydrazide

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Comment

Since some hydrazone derivatives have shown to be potential DNA damaging and mutagenic agents (Okabe *et al.*, 1993), a series of new hydrazone derivatives have been prepared in our laboratory (Shan *et al.*, 2003). As part of the ongoing investigation, the title compound has recently been prepared and its crystal structure is reported here.

The molecular structure of the title compound is shown in Fig. 1. The N2—C8 bond distance of 1.292 (2) Å indicates a typical C═N double bond. The aminophenyl and benzohydrazide moieties located on the opposite sites of the C═N bond, the molecule assumes an E configuration, similat to that found in a related compound, (*E*)-acetylpyrazine 4-nitrophenylhydrazone (Shan *et al.*, 2008). The terminal benzene rings are slightly twisted to the central hydrazide (O1/C7/N1/N2), with dihedral angles of 18.22 (12)° between C1-benzene and hydrazide planes and 27.62 (12)° between aminophenylethylidene and hydrazide planes, indicating the approximately co-planar molecular structure except for methyl H atoms.

The crystal structure contains molecular classic N—H···O hydrogen bonding and weak C—H···N hydrogen bonding (Table 1).

Experimental

Benzohydrazide (0.27 g, 2 mmol) was dissolved in ethanol (10 ml), then acetic acid (0.1 ml) was added to the ethanol solution with stirring. The solution was heated at 333 K for several minutes until the solution cleared. 1-(4-aminophenyl)ethanone (0.27 g, 2 mmol) was then added slowly into the solution, and the mixture was kept at 333 K with continuous stirring for 6 h. After the solution had cooled to room temperature yellow powder crystals appeared. The powder crystals were separated and washed with water three times. Recrystallization from an absolute ethanol yielded well shaped single crystals of the title compound.

Refinement

Methyl H atoms were placed in calculated positions with C—H = 0.96 Å and the torsion angle was refined to fit the electron density, U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were placed in calculated positions with C—H = 0.93 and N—H = 0.86 Å, and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

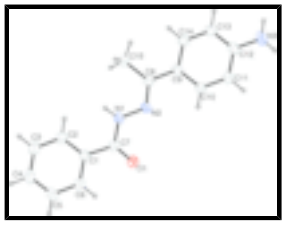

Fig. 1. The molecular structure of the title compound with 50% probability displacement ellipsoids for non-H atoms.

(*E*)-*N*'-[1-(4-Aminophenyl)ethylidene]benzohydrazide

Crystal data

$C_{15}H_{15}N_3O$	F_{000} = 536
M_r = 253.30	D_x = 1.301 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3256 reflections
a = 12.261 (9) Å	θ = 2.0–25.0º
b = 5.324 (4) Å	μ = 0.08 mm^{-1}
c = 19.882 (15) Å	T = 295 (2) K
β = 94.57 (2)º	Prism, yellow
V = 1293.7 (17) Å^3	0.42 × 0.36 × 0.32 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	2303 independent reflections
Radiation source: fine-focus sealed tube	1594 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
Detector resolution: 10.00 pixels mm^{-1}	θ_{max} = 25.2º
T = 295(2) K	θ_{min} = 1.9º
ω scans	h = −14→13
Absorption correction: none	k = −6→6
10914 measured reflections	l = −23→23

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.048	$w = 1/[\sigma^2(F_o^2) + (0.0957P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.156	$(\Delta/\sigma)_{max} < 0.001$
S = 1.06	$\Delta\rho_{max}$ = 0.21 e Å^{-3}

2303 reflections

174 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$\Delta\rho_{min} = -0.15$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.029 (5)

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 $F^2 > \sigma(F^2)$ 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	0.31065 (12)	0.5389 (3)	0.53755 (7)	0.0458 (4)
H1	0.3349	0.3881	0.5344	0.055*
N2	0.21647 (12)	0.6131 (3)	0.49876 (7)	0.0445 (4)
N3	−0.22800 (14)	0.7277 (3)	0.31088 (8)	0.0636 (5)
H3A	−0.2549	0.6375	0.2777	0.076*
H3B	−0.2616	0.8609	0.3223	0.076*
O1	0.33735 (12)	0.9288 (3)	0.58300 (7)	0.0629 (5)
C1	0.45840 (15)	0.6003 (3)	0.62353 (9)	0.0436 (5)
C2	0.51973 (16)	0.3936 (4)	0.60532 (10)	0.0542 (6)
H2	0.5019	0.3119	0.5646	0.065*
C3	0.60765 (18)	0.3099 (4)	0.64827 (12)	0.0653 (6)
H3	0.6489	0.1736	0.6357	0.078*
C4	0.63412 (18)	0.4268 (4)	0.70911 (11)	0.0646 (6)
H4	0.6927	0.3692	0.7375	0.078*
C5	0.57340 (18)	0.6300 (4)	0.72783 (10)	0.0620 (6)
H5	0.5904	0.7084	0.7691	0.074*
C6	0.48743 (16)	0.7162 (4)	0.68502 (9)	0.0545 (6)
H6	0.4479	0.8553	0.6976	0.065*
C7	0.36407 (15)	0.7045 (4)	0.58023 (8)	0.0449 (5)
C8	0.17939 (15)	0.4585 (3)	0.45231 (8)	0.0402 (5)
C9	0.07430 (14)	0.5262 (3)	0.41483 (8)	0.0397 (5)
C10	0.01535 (15)	0.7400 (3)	0.43293 (8)	0.0450 (5)
H10	0.0437	0.8397	0.4685	0.054*
C11	−0.08369 (16)	0.8054 (4)	0.39912 (9)	0.0480 (5)
H11	−0.1199	0.9492	0.4118	0.058*
C12	−0.12988 (15)	0.6578 (4)	0.34612 (9)	0.0477 (5)
C13	−0.07350 (17)	0.4434 (4)	0.32890 (9)	0.0536 (6)

H13	−0.1032	0.3403	0.2944	0.064*
C14	0.02614 (16)	0.3814 (3)	0.36233 (9)	0.0496 (5)
H14	0.0622	0.2378	0.3492	0.060*
C15	0.23698 (17)	0.2176 (3)	0.43604 (10)	0.0544 (6)
H15A	0.3141	0.2481	0.4361	0.082*
H15B	0.2093	0.1587	0.3923	0.082*
H15C	0.2241	0.0929	0.4694	0.082*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0451 (10)	0.0419 (9)	0.0490 (9)	0.0038 (7)	−0.0059 (7)	−0.0028 (7)
N2	0.0436 (10)	0.0446 (10)	0.0437 (8)	0.0004 (7)	−0.0059 (7)	0.0019 (7)
N3	0.0596 (12)	0.0707 (12)	0.0572 (10)	0.0061 (10)	−0.0166 (8)	0.0062 (9)
O1	0.0652 (10)	0.0461 (9)	0.0735 (10)	0.0083 (7)	−0.0176 (8)	−0.0082 (7)
C1	0.0390 (11)	0.0435 (11)	0.0478 (10)	−0.0025 (9)	0.0012 (8)	0.0016 (8)
C2	0.0469 (13)	0.0506 (12)	0.0643 (12)	0.0026 (9)	0.0000 (10)	−0.0059 (10)
C3	0.0582 (14)	0.0520 (13)	0.0851 (16)	0.0127 (11)	0.0029 (12)	0.0019 (11)
C4	0.0526 (14)	0.0656 (15)	0.0735 (15)	0.0092 (11)	−0.0078 (11)	0.0144 (12)
C5	0.0581 (14)	0.0714 (15)	0.0537 (12)	0.0061 (12)	−0.0128 (10)	−0.0033 (11)
C6	0.0530 (13)	0.0545 (13)	0.0545 (12)	0.0089 (10)	−0.0046 (9)	−0.0078 (10)
C7	0.0440 (12)	0.0439 (11)	0.0463 (10)	0.0004 (9)	0.0011 (8)	−0.0029 (8)
C8	0.0467 (11)	0.0343 (10)	0.0395 (9)	−0.0034 (8)	0.0020 (8)	0.0043 (7)
C9	0.0440 (11)	0.0346 (10)	0.0398 (9)	−0.0047 (8)	−0.0011 (8)	0.0047 (7)
C10	0.0487 (12)	0.0419 (11)	0.0433 (10)	−0.0021 (9)	−0.0031 (8)	−0.0043 (8)
C11	0.0474 (12)	0.0476 (12)	0.0487 (10)	0.0028 (9)	0.0030 (9)	0.0027 (9)
C12	0.0485 (12)	0.0492 (12)	0.0442 (10)	−0.0055 (9)	−0.0036 (9)	0.0126 (8)
C13	0.0646 (14)	0.0466 (12)	0.0462 (11)	−0.0057 (10)	−0.0160 (10)	0.0004 (9)
C14	0.0622 (14)	0.0380 (11)	0.0469 (10)	0.0019 (9)	−0.0071 (10)	−0.0020 (8)
C15	0.0584 (13)	0.0437 (12)	0.0588 (12)	0.0055 (10)	−0.0095 (10)	−0.0035 (9)

Geometric parameters (Å, °)

N1—C7	1.355 (2)	C5—H5	0.9300
N1—N2	1.394 (2)	C6—H6	0.9300
N1—H1	0.8600	C8—C9	1.481 (3)
N2—C8	1.292 (2)	C8—C15	1.512 (3)
N3—C12	1.394 (2)	C9—C14	1.391 (2)
N3—H3A	0.8600	C9—C10	1.410 (3)
N3—H3B	0.8600	C10—C11	1.385 (3)
O1—C7	1.241 (2)	C10—H10	0.9300
C1—C6	1.390 (3)	C11—C12	1.398 (3)
C1—C2	1.396 (3)	C11—H11	0.9300
C1—C7	1.493 (3)	C12—C13	1.391 (3)
C2—C3	1.394 (3)	C13—C14	1.384 (3)
C2—H2	0.9300	C13—H13	0.9300
C3—C4	1.376 (3)	C14—H14	0.9300
C3—H3	0.9300	C15—H15A	0.9600
C4—C5	1.381 (3)	C15—H15B	0.9600

C4—H4	0.9300	C15—H15C	0.9600
C5—C6	1.380 (3)		
C7—N1—N2	120.00 (16)	N2—C8—C9	116.56 (16)
C7—N1—H1	120.0	N2—C8—C15	123.33 (17)
N2—N1—H1	120.0	C9—C8—C15	120.10 (16)
C8—N2—N1	116.36 (16)	C14—C9—C10	116.33 (17)
C12—N3—H3A	120.0	C14—C9—C8	122.89 (17)
C12—N3—H3B	120.0	C10—C9—C8	120.74 (16)
H3A—N3—H3B	120.0	C11—C10—C9	121.78 (17)
C6—C1—C2	118.19 (18)	C11—C10—H10	119.1
C6—C1—C7	118.33 (17)	C9—C10—H10	119.1
C2—C1—C7	123.48 (17)	C10—C11—C12	120.77 (18)
C3—C2—C1	119.9 (2)	C10—C11—H11	119.6
C3—C2—H2	120.0	C12—C11—H11	119.6
C1—C2—H2	120.0	C13—C12—N3	121.40 (18)
C4—C3—C2	120.7 (2)	C13—C12—C11	117.86 (18)
C4—C3—H3	119.6	N3—C12—C11	120.73 (19)
C2—C3—H3	119.6	C14—C13—C12	120.99 (17)
C3—C4—C5	119.8 (2)	C14—C13—H13	119.5
C3—C4—H4	120.1	C12—C13—H13	119.5
C5—C4—H4	120.1	C13—C14—C9	122.26 (18)
C6—C5—C4	119.8 (2)	C13—C14—H14	118.9
C6—C5—H5	120.1	C9—C14—H14	118.9
C4—C5—H5	120.1	C8—C15—H15A	109.5
C5—C6—C1	121.62 (19)	C8—C15—H15B	109.5
C5—C6—H6	119.2	H15A—C15—H15B	109.5
C1—C6—H6	119.2	C8—C15—H15C	109.5
O1—C7—N1	122.51 (17)	H15A—C15—H15C	109.5
O1—C7—C1	121.83 (16)	H15B—C15—H15C	109.5
N1—C7—C1	115.66 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3B···O1^{i}	0.86	2.44	3.169 (3)	143
C15—H15C···N2^{ii}	0.96	2.62	3.468 (3)	147

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

Fig. 1