Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-[1-(4-Chlorophenyl)ethylidene]-acetohydrazide

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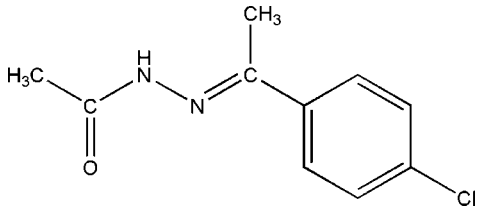
Received 15 October 2010; accepted 20 October 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.164; data-to-parameter ratio = 16.6.

In the title compound, $C_{10}H_{11}ClN_2O$, the dihedral angle between the acetohydrazide group and the aromatic ring is 33.76 (9)°. In the crystal, inversion dimers linked by pairs of N—H···O hydrogen bonds generate $R_2^2(8)$ loops.

Related literature

For a related structure, see: Li & Jian (2008).



Experimental

Crystal data

$C_{10}H_{11}ClN_2O$
M_r = 210.66
Monoclinic, $P2_1/c$
a = 15.944 (3) Å
b = 5.0061 (10) Å
c = 13.950 (3) Å
β = 109.45 (3)°
V = 1049.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
9225 measured reflections
2368 independent reflections
1840 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.164
S = 1.22
2368 reflections
143 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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}	0.93 (2)	2.02 (2)	2.9384 (18)	170.3 (18)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors would like to thank the National Natural Science Foundation of Shandong Province (Y2008B29) and Yuandu Scholar of Weifang City.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5687).

References

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supplementary materials

Acta Cryst. (2010). E**66**, o2941 [**doi:10.1107/S1600536810042546**]

N'-[1-(4-Chlorophenyl)ethylidene]acetohydrazide

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Experimental

A mixture of 4-fluorobenzophenone (0.02 mol) and acethydrazide (0.02 mol) was stirred in refluxing ethanol(30 ml) for 2 h to afford the title compound (yield 82%). Yellow bars of (I) were obtained by recrystallization from acetic ether at room temperature.

Refinement

All H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H and N—H distances in the range 0.93–0.97Å and 0.86 Å, and with $U_{iso}(H) = 1.2U_{eq}$ of the parent atoms.

Figures

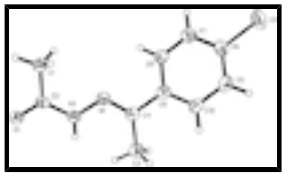

Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level.

N'-[1-(4-Chlorophenyl)ethylidene]acetohydrazide

Crystal data

$C_{10}H_{11}ClN_2O$	$F(000) = 440$
$M_r = 210.66$	$D_x = 1.333$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2368 reflections
$a = 15.944$ (3) Å	$\theta = 3.1$–$27.5°$
$b = 5.0061$ (10) Å	$\mu = 0.33$ mm^{-1}
$c = 13.950$ (3) Å	$T = 293$ K
$\beta = 109.45$ (3)°	Bar, yellow
$V = 1049.9$ (4) Å^3	0.25 × 0.20 × 0.20 mm
$Z = 4$	

Data collection

Bruker SMART CCD diffractometer	1840 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.028$
graphite	$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$

phi and ω scans	$h = -20 \rightarrow 20$
9225 measured reflections	$k = -6 \rightarrow 6$
2368 independent reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.046$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.164$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.22$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
2368 reflections	$(\Delta/\sigma)_{max} < 0.001$
143 parameters	$\Delta\rho_{max} = 0.29$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.22$ e Å^{-3}

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}
Cl1	0.05552 (4)	0.51605 (12)	0.20233 (5)	0.0784 (3)
O1	0.58233 (7)	−0.3084 (2)	0.08042 (9)	0.0515 (3)
N2	0.43948 (8)	−0.2513 (3)	0.06514 (10)	0.0437 (3)
N1	0.37755 (9)	−0.1121 (3)	0.09450 (10)	0.0450 (3)
C4	0.29443 (11)	−0.1619 (3)	0.04835 (12)	0.0449 (4)
C5	0.23285 (11)	−0.0057 (3)	0.08658 (12)	0.0449 (4)
C2	0.52624 (10)	−0.1844 (3)	0.10492 (11)	0.0409 (3)
C8	0.12309 (12)	0.3099 (3)	0.15743 (15)	0.0544 (4)
C7	0.20770 (13)	0.2495 (4)	0.22141 (14)	0.0598 (5)
H7A	0.2280	0.3142	0.2877	0.072*
C6	0.26121 (11)	0.0927 (4)	0.18559 (13)	0.0544 (4)
H6A	0.3181	0.0507	0.2287	0.065*
C10	0.14651 (12)	0.0543 (4)	0.02497 (14)	0.0572 (5)
H10A	0.1251	−0.0132	−0.0408	0.069*

C1	0.55118 (11)	0.0442 (3)	0.17832 (14)	0.0517 (4)
H1B	0.6144	0.0700	0.2004	0.078*
H1C	0.5332	0.0054	0.2360	0.078*
H1D	0.5219	0.2036	0.1456	0.078*
C9	0.09182 (12)	0.2137 (4)	0.06054 (15)	0.0620 (5)
H9A	0.0344	0.2544	0.0186	0.074*
C3	0.25881 (16)	−0.3524 (5)	−0.0385 (2)	0.0663 (6)
H2A	0.4257 (13)	−0.391 (4)	0.0186 (17)	0.062 (5)*
H3A	0.197 (2)	−0.372 (5)	−0.064 (2)	0.106 (9)*
H3B	0.279 (3)	−0.503 (7)	−0.022 (3)	0.155 (16)*
H3C	0.278 (2)	−0.321 (6)	−0.094 (2)	0.115 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0715 (4)	0.0887 (5)	0.0850 (5)	0.0221 (3)	0.0396 (3)	0.0014 (3)
O1	0.0511 (6)	0.0533 (6)	0.0489 (7)	0.0016 (5)	0.0151 (5)	−0.0108 (5)
N2	0.0479 (7)	0.0422 (7)	0.0401 (7)	0.0027 (6)	0.0134 (5)	−0.0058 (5)
N1	0.0475 (7)	0.0469 (7)	0.0399 (7)	0.0038 (6)	0.0137 (5)	−0.0018 (5)
C4	0.0495 (8)	0.0424 (8)	0.0417 (8)	−0.0018 (6)	0.0138 (6)	0.0016 (6)
C5	0.0462 (9)	0.0451 (8)	0.0414 (9)	−0.0024 (6)	0.0119 (7)	0.0029 (6)
C2	0.0510 (8)	0.0378 (7)	0.0325 (7)	0.0033 (6)	0.0122 (6)	0.0004 (5)
C8	0.0520 (9)	0.0554 (9)	0.0615 (11)	0.0043 (7)	0.0267 (8)	0.0037 (8)
C7	0.0601 (10)	0.0706 (11)	0.0469 (10)	0.0085 (9)	0.0154 (8)	−0.0030 (8)
C6	0.0501 (9)	0.0641 (10)	0.0442 (9)	0.0074 (8)	0.0092 (7)	−0.0016 (7)
C10	0.0466 (9)	0.0701 (11)	0.0496 (10)	−0.0019 (8)	0.0089 (7)	−0.0065 (8)
C1	0.0571 (10)	0.0488 (9)	0.0491 (10)	−0.0064 (7)	0.0175 (7)	−0.0115 (7)
C9	0.0429 (8)	0.0705 (11)	0.0663 (12)	0.0032 (8)	0.0097 (8)	0.0008 (9)
C3	0.0595 (12)	0.0661 (13)	0.0687 (14)	−0.0060 (10)	0.0154 (10)	−0.0225 (10)

Geometric parameters (Å, °)

Cl1—C8	1.7512 (17)	C7—C6	1.370 (2)
O1—C2	1.2269 (18)	C7—H7A	0.9300
N2—C2	1.350 (2)	C6—H6A	0.9300
N2—N1	1.3773 (17)	C10—C9	1.390 (3)
N2—H2A	0.93 (2)	C10—H10A	0.9300
N1—C4	1.290 (2)	C1—H1B	0.9600
C4—C5	1.486 (2)	C1—H1C	0.9600
C4—C3	1.497 (2)	C1—H1D	0.9600
C5—C10	1.391 (2)	C9—H9A	0.9300
C5—C6	1.392 (2)	C3—H3A	0.93 (3)
C2—C1	1.498 (2)	C3—H3B	0.83 (4)
C8—C9	1.363 (3)	C3—H3C	0.94 (3)
C8—C7	1.381 (3)		
C2—N2—N1	119.36 (13)	C7—C6—H6A	119.1
C2—N2—H2A	116.5 (12)	C5—C6—H6A	119.1
N1—N2—H2A	124.2 (12)	C9—C10—C5	120.84 (17)

C4—N1—N2	118.22 (13)	C9—C10—H10A	119.6
N1—C4—C5	114.25 (13)	C5—C10—H10A	119.6
N1—C4—C3	125.23 (16)	C2—C1—H1B	109.5
C5—C4—C3	120.50 (15)	C2—C1—H1C	109.5
C10—C5—C6	117.66 (16)	H1B—C1—H1C	109.5
C10—C5—C4	121.86 (15)	C2—C1—H1D	109.5
C6—C5—C4	120.46 (14)	H1B—C1—H1D	109.5
O1—C2—N2	120.14 (14)	H1C—C1—H1D	109.5
O1—C2—C1	121.64 (14)	C8—C9—C10	119.41 (16)
N2—C2—C1	118.22 (14)	C8—C9—H9A	120.3
C9—C8—C7	121.30 (16)	C10—C9—H9A	120.3
C9—C8—Cl1	119.82 (14)	C4—C3—H3A	116.6 (17)
C7—C8—Cl1	118.88 (15)	C4—C3—H3B	110 (3)
C6—C7—C8	118.87 (17)	H3A—C3—H3B	106 (3)
C6—C7—H7A	120.6	C4—C3—H3C	115.3 (18)
C8—C7—H7A	120.6	H3A—C3—H3C	107 (2)
C7—C6—C5	121.89 (16)	H3B—C3—H3C	101 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O1^{i}	0.93 (2)	2.02 (2)	2.9384 (18)	170.3 (18)

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

Fig. 1