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

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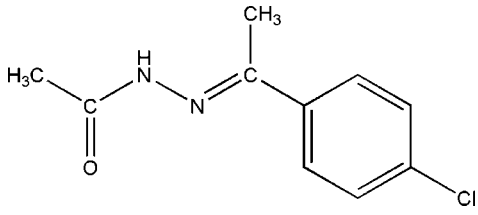
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.164; data-to-parameter ratio = 16.6.

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*.

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

References

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

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

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

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S1. 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.

S2. 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.

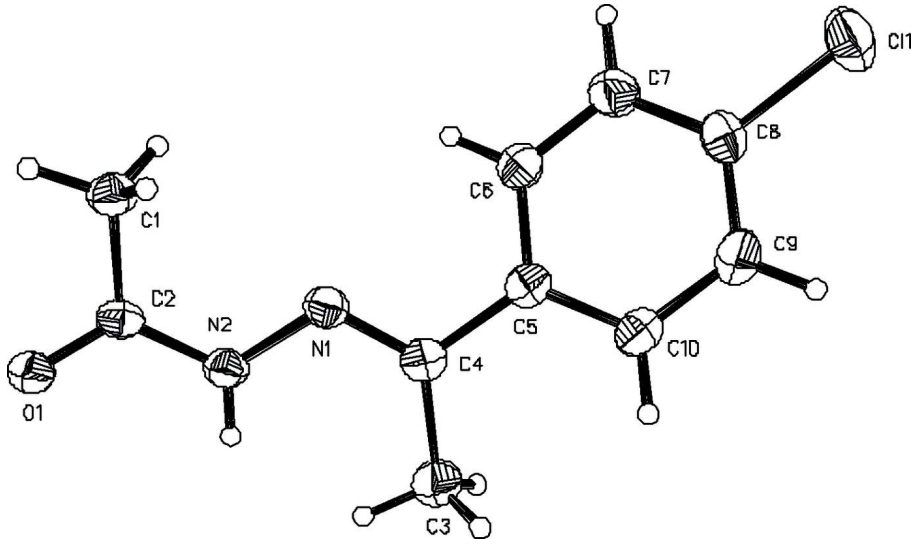

Figure 1

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

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

Crystal data

$C_{10}H_{11}ClN_2O$
M_r = 210.66
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
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
F(000) = 440
D_x = 1.333 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2368 reflections
θ = 3.1–27.5°
μ = 0.33 mm^{-1}

T = 293 K
Bar, yellow

0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
9225 measured reflections
2368 independent reflections

1840 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −20→20
k = −6→6
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.164
S = 1.22
2368 reflections
143 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −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 (Å²)

	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, º)

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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.93 (2)	2.02 (2)	2.9384 (18)	170.3 (18)

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