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

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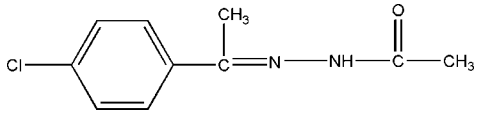
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.055; wR factor = 0.191; data-to-parameter ratio = 13.8.

The title compound, $C_{11}H_{14}ClN_2O$, was prepared by the reaction between *p*-chlorohypnone and acetohydrazide. The asymmetric unit consists of two crystallographically independent molecules. Symmetry-related molecules form two N—H···O and weak C—H···O hydrogen-bonded chains. Weak interactions between the dimers stabilize the crystal packing.

Related literature

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



Experimental

Crystal data

$C_{11}H_{14}ClN_2O$
M_r = 190.24
Monoclinic, $P2_1/n$
a = 7.2462 (14) Å
b = 25.710 (5) Å
c = 11.616 (2) Å
β = 105.159 (4)°
V = 2088.8 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
10760 measured reflections
3691 independent reflections
1849 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.191
S = 1.05
3691 reflections
268 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 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
N2—H2A···O2^{i}	0.898 (11)	2.076 (11)	2.965 (3)	170 (3)
N4—H4A···O1^{ii}	0.900 (14)	2.093 (13)	2.976 (3)	167 (3)
C9—H9C···O2^{i}	0.96	2.39	3.199 (4)	141
C20—H20C···O1^{ii}	0.96	2.60	3.243 (4)	125

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

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: AT2316).

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supplementary materials

Acta Cryst. (2007). E**63**, o3124 [**doi:10.1107/S1600536807026736**]

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

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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.

The independent molecules in the asymmetric unit (Fig.1) are linked together to form the first two dimer by N2—H2A···O2^{i} and weak C9—H9C···O2^{i} hydrogen bonds, and the second two dimer N4—H4A···O1^{ii} and C20—H20C···O1^{ii} hydrogen bonds [symmetry codes: (i) *x*, *y* − 1, *z* − 1; (ii) *x*, *y* + 1, *z* + 1] (Table 2, Fig. 2). The structure is stabilized by weak-interactions between the dimers.

Experimental

A mixture of the *p*-chlorohypnone (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 atoms bound to the N atoms were 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 = 0.93–0.96 Å, and with $U_{iso} = 1.2U_{eq}(C_{aromatic})$ or $1.5U_{eq}(C_{methyl})$.

Figures

Fig. 1. View of two independent molecules of the title compound in the asymmetric unit. Displacement ellipsoids are drawn at the 30% probability level.

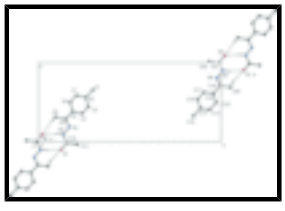


Fig. 2. A view of the N—H.·O and weak C—H.·O hydrogen-bonded dimers. [Symmetry codes: (*a*) *x*, *y* − 1, *z* − 1; (*b*) *x*, *y* + 1, *z* + 1]. For clarity, the hydrogen atoms not involving hydrogen bonding are omitted.

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

Crystal data

$C_{11}H_{14}ClN_2O$ $Z = 8$

M_r = 190.24	F_{000} = 816
Monoclinic, $P2_1/n$	D_x = 1.210 Mg m^{-3}
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.2462 (14) Å	θ = 1.6–25.0º
b = 25.710 (5) Å	μ = 0.08 mm^{-1}
c = 11.616 (2) Å	T = 294 (2) K
β = 105.159 (4)º	Block, colourless
V = 2088.8 (7) Å^3	0.22 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer	1849 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.054
Monochromator: graphite	θ_{max} = 25.0º
T = 294(2) K	θ_{min} = 1.6º
φ and ω scans	h = −5→8
Absorption correction: none	k = −30→29
10760 measured reflections	l = −13→9
3691 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
$R[F^2 > 2\sigma(F^2)]$ = 0.055	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.191	$w = 1/[\sigma^2(F_o^2) + (0.0932P)^2 + 0.0086P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.002
3691 reflections	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
268 parameters	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
2 restraints	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: 0.034 (4)

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	0.2533 (3)	0.12503 (8)	−0.0950 (2)	0.0807 (7)
O2	0.2528 (3)	1.01951 (8)	1.0905 (2)	0.0770 (7)
N1	0.2490 (3)	0.16788 (8)	0.1870 (2)	0.0514 (6)
N2	0.2523 (3)	0.13483 (9)	0.0946 (2)	0.0552 (6)
N3	0.2353 (3)	0.97667 (8)	0.8058 (2)	0.0555 (7)
N4	0.2507 (4)	1.00931 (9)	0.9010 (2)	0.0596 (7)
C1	0.2288 (4)	0.29725 (12)	0.6570 (3)	0.0724 (10)
H1A	0.3500	0.2980	0.7156	0.109*
H1B	0.1306	0.2873	0.6943	0.109*
H1C	0.2008	0.3311	0.6221	0.109*
C2	0.2367 (4)	0.25878 (11)	0.5618 (3)	0.0526 (7)
C3	0.1961 (4)	0.27272 (11)	0.4439 (3)	0.0597 (8)
H3	0.1633	0.3070	0.4227	0.072*
C4	0.2024 (4)	0.23771 (10)	0.3567 (3)	0.0547 (8)
H4	0.1736	0.2488	0.2778	0.066*
C5	0.2503 (3)	0.18636 (10)	0.3828 (2)	0.0448 (7)
C6	0.2918 (4)	0.17274 (12)	0.5007 (3)	0.0648 (9)
H6	0.3254	0.1385	0.5224	0.078*
C7	0.2851 (4)	0.20834 (12)	0.5880 (3)	0.0663 (9)
H7	0.3145	0.1975	0.6672	0.080*
C8	0.2555 (3)	0.14834 (10)	0.2888 (3)	0.0470 (7)
C9	0.2613 (5)	0.09175 (10)	0.3161 (3)	0.0760 (10)
H9A	0.1333	0.0789	0.3040	0.114*
H9B	0.3310	0.0862	0.3976	0.114*
H9C	0.3233	0.0736	0.2644	0.114*
C10	0.2411 (4)	0.15422 (11)	−0.0140 (3)	0.0545 (8)
C11	0.2128 (4)	0.21087 (11)	−0.0330 (3)	0.0631 (9)
H11A	0.3142	0.2292	0.0217	0.095*
H11B	0.0924	0.2208	−0.0196	0.095*
H11C	0.2135	0.2194	−0.1133	0.095*
C12	0.1844 (5)	0.84704 (13)	0.3241 (3)	0.0907 (12)
H12A	0.0784	0.8565	0.2588	0.136*
H12B	0.1631	0.8130	0.3522	0.136*
H12C	0.2996	0.8469	0.2980	0.136*
C13	0.2035 (4)	0.88583 (12)	0.4237 (3)	0.0633 (8)
C14	0.2189 (4)	0.93726 (13)	0.4059 (3)	0.0706 (9)
H14	0.2179	0.9492	0.3302	0.085*
C15	0.2361 (4)	0.97266 (12)	0.4971 (3)	0.0661 (9)
H15	0.2458	1.0079	0.4811	0.079*
C16	0.2394 (4)	0.95761 (10)	0.6107 (2)	0.0481 (7)
C17	0.2238 (5)	0.90498 (11)	0.6279 (3)	0.0704 (9)
H17	0.2249	0.8928	0.7035	0.085*

C18	0.2067 (5)	0.87037 (12)	0.5374 (3)	0.0764 (10)
H18	0.1970	0.8351	0.5528	0.092*
C19	0.2579 (4)	0.99517 (10)	0.7081 (3)	0.0517 (8)
C20	0.3030 (5)	1.05082 (11)	0.6893 (3)	0.0796 (10)
H20A	0.1862	1.0702	0.6638	0.119*
H20B	0.3722	1.0528	0.6293	0.119*
H20C	0.3795	1.0651	0.7626	0.119*
C21	0.2446 (4)	0.99006 (12)	1.0067 (3)	0.0593 (8)
C22	0.2293 (5)	0.93300 (11)	1.0181 (3)	0.0763 (10)
H22A	0.3429	0.9167	1.0073	0.114*
H22B	0.1202	0.9205	0.9584	0.114*
H22C	0.2150	0.9247	1.0959	0.114*
H2A	0.262 (4)	0.1001 (4)	0.102 (3)	0.077 (10)*
H4A	0.232 (4)	1.0439 (5)	0.894 (3)	0.100 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.132 (2)	0.0583 (13)	0.0566 (16)	0.0028 (12)	0.0340 (13)	−0.0090 (12)
O2	0.1214 (19)	0.0576 (13)	0.0579 (15)	−0.0037 (11)	0.0338 (12)	−0.0112 (12)
N1	0.0608 (15)	0.0450 (13)	0.0508 (17)	−0.0039 (10)	0.0190 (11)	−0.0075 (12)
N2	0.0782 (17)	0.0394 (15)	0.0508 (17)	−0.0038 (11)	0.0220 (12)	−0.0043 (13)
N3	0.0723 (16)	0.0459 (14)	0.0515 (18)	−0.0001 (11)	0.0218 (12)	−0.0059 (13)
N4	0.0869 (18)	0.0422 (15)	0.0548 (19)	−0.0023 (12)	0.0278 (13)	−0.0080 (14)
C1	0.078 (2)	0.073 (2)	0.066 (2)	0.0039 (16)	0.0180 (16)	−0.0181 (18)
C2	0.0531 (17)	0.0536 (18)	0.050 (2)	−0.0021 (13)	0.0117 (13)	−0.0085 (15)
C3	0.075 (2)	0.0426 (17)	0.063 (2)	0.0058 (13)	0.0220 (16)	0.0006 (16)
C4	0.0693 (19)	0.0496 (17)	0.0450 (19)	0.0027 (13)	0.0148 (14)	0.0067 (15)
C5	0.0486 (16)	0.0420 (16)	0.0453 (19)	−0.0004 (11)	0.0150 (13)	0.0022 (14)
C6	0.095 (2)	0.0449 (18)	0.053 (2)	0.0042 (15)	0.0160 (16)	0.0040 (16)
C7	0.090 (2)	0.064 (2)	0.043 (2)	0.0047 (16)	0.0125 (16)	0.0036 (16)
C8	0.0528 (17)	0.0423 (16)	0.046 (2)	−0.0044 (11)	0.0136 (13)	0.0034 (14)
C9	0.124 (3)	0.0448 (18)	0.060 (2)	−0.0002 (16)	0.0245 (19)	0.0017 (16)
C10	0.071 (2)	0.0454 (18)	0.050 (2)	−0.0032 (13)	0.0206 (15)	−0.0030 (16)
C11	0.083 (2)	0.0534 (19)	0.054 (2)	0.0039 (15)	0.0191 (16)	0.0022 (15)
C12	0.124 (3)	0.080 (2)	0.066 (3)	0.012 (2)	0.022 (2)	−0.021 (2)
C13	0.077 (2)	0.058 (2)	0.056 (2)	0.0105 (15)	0.0178 (16)	−0.0055 (17)
C14	0.098 (2)	0.071 (2)	0.046 (2)	0.0070 (17)	0.0255 (17)	0.0062 (18)
C15	0.097 (2)	0.0483 (19)	0.059 (2)	0.0055 (15)	0.0306 (18)	0.0085 (16)
C16	0.0583 (17)	0.0414 (16)	0.049 (2)	0.0051 (12)	0.0223 (14)	0.0044 (14)
C17	0.119 (3)	0.0452 (19)	0.055 (2)	0.0039 (16)	0.0372 (19)	0.0044 (16)
C18	0.120 (3)	0.0487 (19)	0.064 (3)	−0.0007 (17)	0.032 (2)	−0.0041 (18)
C19	0.0629 (19)	0.0452 (16)	0.051 (2)	0.0008 (12)	0.0220 (15)	0.0063 (14)
C20	0.124 (3)	0.0492 (19)	0.077 (3)	−0.0136 (17)	0.046 (2)	−0.0042 (17)
C21	0.078 (2)	0.0488 (19)	0.056 (2)	−0.0018 (14)	0.0250 (16)	−0.0054 (17)
C22	0.123 (3)	0.052 (2)	0.060 (2)	−0.0063 (17)	0.033 (2)	−0.0012 (16)

Geometric parameters (Å, °)

O1—C10	1.225 (3)	C9—H9C	0.9600
O2—C21	1.223 (3)	C10—C11	1.479 (4)
N1—C8	1.274 (3)	C11—H11A	0.9600
N1—N2	1.374 (3)	C11—H11B	0.9600
N2—C10	1.339 (4)	C11—H11C	0.9600
N2—H2A	0.897 (10)	C12—C13	1.505 (4)
N3—C19	1.280 (3)	C12—H12A	0.9600
N3—N4	1.369 (3)	C12—H12B	0.9600
N4—C21	1.335 (4)	C12—H12C	0.9600
N4—H4A	0.900 (10)	C13—C14	1.347 (4)
C1—C2	1.495 (4)	C13—C18	1.374 (4)
C1—H1A	0.9600	C14—C15	1.378 (4)
C1—H1B	0.9600	C14—H14	0.9300
C1—H1C	0.9600	C15—C16	1.369 (4)
C2—C7	1.357 (4)	C15—H15	0.9300
C2—C3	1.372 (4)	C16—C17	1.377 (4)
C3—C4	1.364 (4)	C16—C19	1.467 (4)
C3—H3	0.9300	C17—C18	1.359 (4)
C4—C5	1.379 (3)	C17—H17	0.9300
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.368 (4)	C19—C20	1.496 (4)
C5—C8	1.474 (4)	C20—H20A	0.9600
C6—C7	1.377 (4)	C20—H20B	0.9600
C6—H6	0.9300	C20—H20C	0.9600
C7—H7	0.9300	C21—C22	1.480 (4)
C8—C9	1.487 (4)	C22—H22A	0.9600
C9—H9A	0.9600	C22—H22B	0.9600
C9—H9B	0.9600	C22—H22C	0.9600
C8—N1—N2	118.5 (2)	H11A—C11—H11B	109.5
C10—N2—N1	119.8 (2)	C10—C11—H11C	109.5
C10—N2—H2A	116 (2)	H11A—C11—H11C	109.5
N1—N2—H2A	124 (2)	H11B—C11—H11C	109.5
C19—N3—N4	119.1 (2)	C13—C12—H12A	109.5
C21—N4—N3	120.0 (3)	C13—C12—H12B	109.5
C21—N4—H4A	114 (2)	H12A—C12—H12B	109.5
N3—N4—H4A	123 (2)	C13—C12—H12C	109.5
C2—C1—H1A	109.5	H12A—C12—H12C	109.5
C2—C1—H1B	109.5	H12B—C12—H12C	109.5
H1A—C1—H1B	109.5	C14—C13—C18	116.7 (3)
C2—C1—H1C	109.5	C14—C13—C12	121.8 (3)
H1A—C1—H1C	109.5	C18—C13—C12	121.5 (3)
H1B—C1—H1C	109.5	C13—C14—C15	121.7 (3)
C7—C2—C3	116.7 (3)	C13—C14—H14	119.1
C7—C2—C1	121.6 (3)	C15—C14—H14	119.1
C3—C2—C1	121.7 (3)	C16—C15—C14	122.0 (3)
C4—C3—C2	121.9 (3)	C16—C15—H15	119.0

C4—C3—H3	119.0	C14—C15—H15	119.0
C2—C3—H3	119.0	C15—C16—C17	115.9 (3)
C3—C4—C5	121.6 (3)	C15—C16—C19	122.2 (3)
C3—C4—H4	119.2	C17—C16—C19	122.0 (3)
C5—C4—H4	119.2	C18—C17—C16	121.7 (3)
C6—C5—C4	116.2 (3)	C18—C17—H17	119.1
C6—C5—C8	122.0 (2)	C16—C17—H17	119.1
C4—C5—C8	121.7 (3)	C17—C18—C13	122.0 (3)
C5—C6—C7	121.8 (3)	C17—C18—H18	119.0
C5—C6—H6	119.1	C13—C18—H18	119.0
C7—C6—H6	119.1	N3—C19—C16	115.6 (2)
C2—C7—C6	121.8 (3)	N3—C19—C20	124.7 (3)
C2—C7—H7	119.1	C16—C19—C20	119.7 (3)
C6—C7—H7	119.1	C19—C20—H20A	109.5
N1—C8—C5	115.1 (2)	C19—C20—H20B	109.5
N1—C8—C9	125.2 (3)	H20A—C20—H20B	109.5
C5—C8—C9	119.7 (3)	C19—C20—H20C	109.5
C8—C9—H9A	109.5	H20A—C20—H20C	109.5
C8—C9—H9B	109.5	H20B—C20—H20C	109.5
H9A—C9—H9B	109.5	O2—C21—N4	119.8 (3)
C8—C9—H9C	109.5	O2—C21—C22	122.1 (3)
H9A—C9—H9C	109.5	N4—C21—C22	118.1 (3)
H9B—C9—H9C	109.5	C21—C22—H22A	109.5
O1—C10—N2	119.8 (3)	C21—C22—H22B	109.5
O1—C10—C11	121.6 (3)	H22A—C22—H22B	109.5
N2—C10—C11	118.6 (3)	C21—C22—H22C	109.5
C10—C11—H11A	109.5	H22A—C22—H22C	109.5
C10—C11—H11B	109.5	H22B—C22—H22C	109.5
C8—N1—N2—C10	178.4 (2)	N1—N2—C10—C11	−3.9 (4)
C19—N3—N4—C21	−174.0 (3)	C18—C13—C14—C15	−0.3 (5)
C7—C2—C3—C4	0.5 (4)	C12—C13—C14—C15	179.9 (3)
C1—C2—C3—C4	−179.8 (3)	C13—C14—C15—C16	0.3 (5)
C2—C3—C4—C5	−0.1 (4)	C14—C15—C16—C17	−0.2 (4)
C3—C4—C5—C6	−0.3 (4)	C14—C15—C16—C19	179.9 (3)
C3—C4—C5—C8	179.4 (2)	C15—C16—C17—C18	0.2 (4)
C4—C5—C6—C7	0.3 (4)	C19—C16—C17—C18	−180.0 (3)
C8—C5—C6—C7	−179.4 (3)	C16—C17—C18—C13	−0.2 (5)
C3—C2—C7—C6	−0.5 (4)	C14—C13—C18—C17	0.3 (5)
C1—C2—C7—C6	179.8 (3)	C12—C13—C18—C17	−179.9 (3)
C5—C6—C7—C2	0.1 (5)	N4—N3—C19—C16	179.9 (2)
N2—N1—C8—C5	−179.7 (2)	N4—N3—C19—C20	0.6 (4)
N2—N1—C8—C9	−1.7 (4)	C15—C16—C19—N3	171.7 (3)
C6—C5—C8—N1	−167.5 (2)	C17—C16—C19—N3	−8.2 (4)
C4—C5—C8—N1	12.8 (4)	C15—C16—C19—C20	−9.1 (4)
C6—C5—C8—C9	14.4 (4)	C17—C16—C19—C20	171.1 (3)
C4—C5—C8—C9	−165.3 (3)	N3—N4—C21—O2	−177.8 (3)
N1—N2—C10—O1	176.5 (2)	N3—N4—C21—C22	2.6 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O2^{i}	0.898 (11)	2.076 (11)	2.965 (3)	170 (3)
N4—H4A···O1^{ii}	0.900 (14)	2.093 (13)	2.976 (3)	167 (3)
C9—H9C···O2^{i}	0.96	2.39	3.199 (4)	141
C20—H20C···O1^{ii}	0.96	2.60	3.243 (4)	125

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

Fig. 1

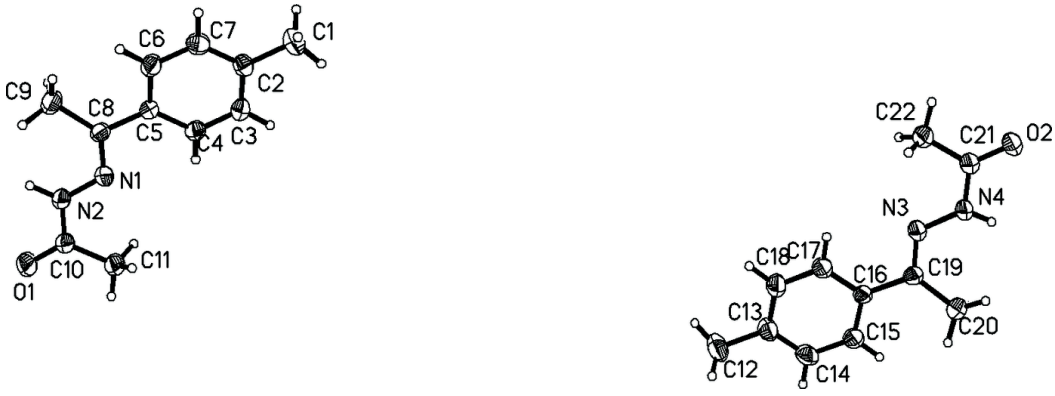
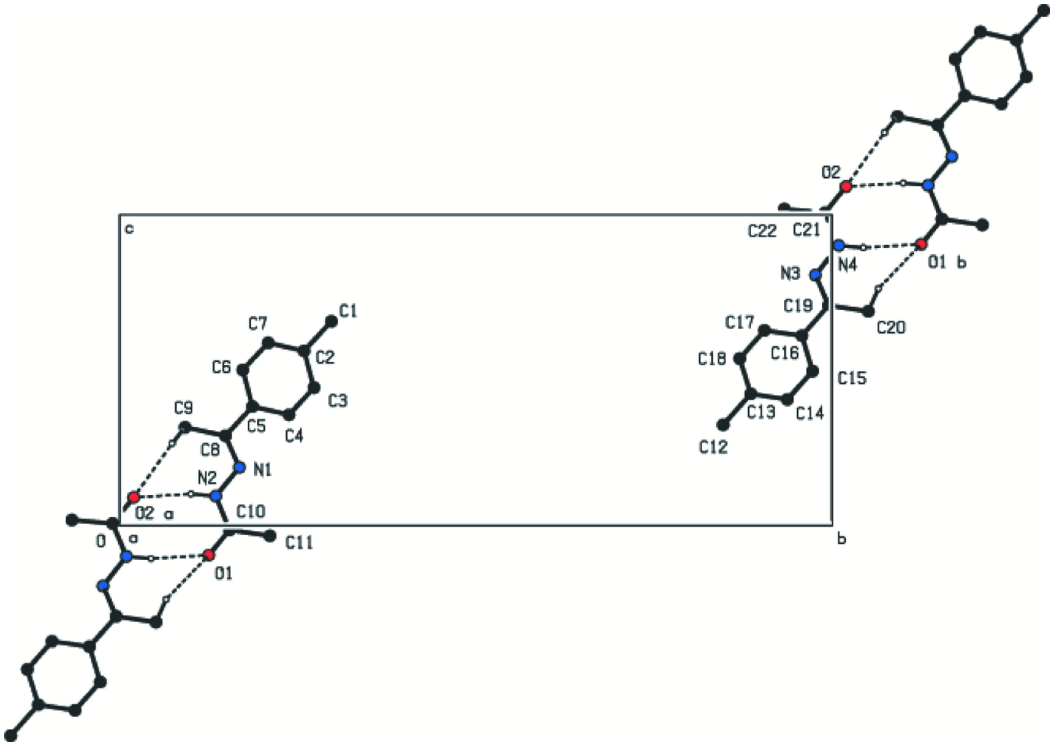

C6
C7
C1
C9
C8
C2
C5
C4
C3
N1
N2
C10
C11
O1
C22
C21
O2
N3
N4
C18
C17
C16
C19
C13
C15
C20
C12
C14

Fig. 2


c
C22
C21
O2
N3
N4
O1 b
C19
C17
C20
C18
C16
C15
C13
C14
C12
b
C7
C1
C6
C2
C3
C9
C5
C4
C8
N1
N2
O2 a
C10
O
a
C11
O1