Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-*N*′-[4-(4-Chlorobenzoyloxy)-3-methoxybenzylidene]isonicotinohydrazide

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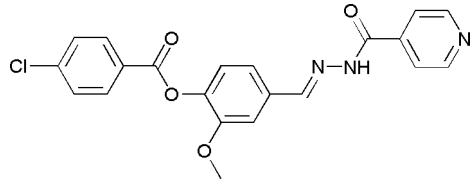
Received 4 September 2007; accepted 4 September 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.111; data-to-parameter ratio = 15.4.

In the title compound, $C_{21}H_{16}ClN_3O_4$, the vanillin group makes dihedral angles of 83.04 (6) and 53.42 (6)° with the mean planes of the terminal chlorobenzene and pyridine rings, respectively. The packing is stabilized by intermolecular N—H···O hydrogen bonds and weak C—H···O interactions that link adjacent molecules into chains.

Related literature

For general background, see: Kahwa *et al.* (1986); Santos *et al.* (2001). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{21}H_{16}ClN_3O_4$
M_r = 409.82
Monoclinic, $P2_1/c$
a = 21.746 (6) Å
b = 12.011 (3) Å
c = 7.700 (2) Å
β = 99.472 (5)°
V = 1983.8 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 294 (2) K
0.16 × 0.16 × 0.14 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.938, T_{max} = 0.969
10889 measured reflections
4047 independent reflections
2457 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.111
S = 1.02
4047 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O4^{i}	0.86	2.03	2.807 (2)	150
C19—H19···O1^{ii}	0.93	2.52	3.420 (3)	162

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The project was supported by the Foundation of the Education Department of Hebei Province (grant No. 606022).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2532).

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 doi:10.1107/S1600536807043395

supplementary materials

Acta Cryst. (2007). E**63**, o4013 [**doi:10.1107/S1600536807043395**]

(*E*)-*N*'-[4-(4-Chlorobenzoyloxy)-3-methoxybenzylidene]isonicotinohydrazide

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Comment

The synthesis and structure of Schiff bases have attracted much attention in biology and chemistry (Kahwa *et al.*, 1986). One aim is to develop protein and enzyme mimics (Santos *et al.*, 2001). As part of an investigation of the coordination properties of Schiff bases functioning as ligands, we report the synthesis and structure of the title compound, (I).

In (I) (Fig. 1), the vanillin group (C8—C13/C15/O2/O3) is nearly planar, with an r.m.s. deviation for fitted atoms of 0.0283 Å. This plane makes dihedral angles of 53.42 (6)° and 83.04 (6)° with the pyridine ring (C17—C21/N3) and the terminal benzene ring (C1—C6), respectively. The dihedral angle between the pyridine ring and the benzene ring is 43.89 (10)°. Otherwise, all bond lengths and angles are within their normal ranges (Allen *et al.*, 1987).

The crystal packing is stabilized by intermolecular N—H···O and C—H···O hydrogen bonds that link adjacent molecules into one-dimensional extended (Table 1, Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 4-formyl-2-methoxyphenyl 4-chlorobenzoate (2.91 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of isonicotinohydrazide (1.37 g, 10 mmol) and the mixture stirred at 350 K for 5 h under nitrogen, giving a white precipitate. The product was isolated, recrystallized from ethanol and then dried in a vacuum to give the pure compound in 75% yield. Colourless blocks of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Refinement

The H atoms were included in calculated positions and refined using a riding model approximation. Constrained C—H and N—H bond lengths and isotropic U parameters: 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2—H; 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl C—H; 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N) for imino N—H.

Figures

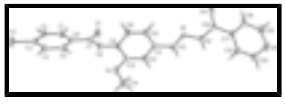

Fig. 1. The structure of (I) with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

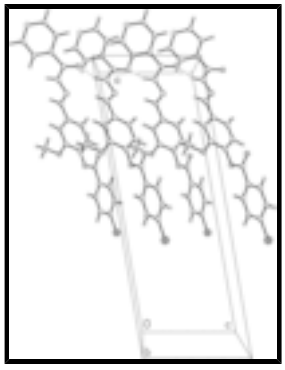

Fig. 2. Partial packing diagram for (I), with H bonds drawn as dashed lines.

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Crystal data

$C_{21}H_{16}ClN_3O_4$	F_{000} = 848
M_r = 409.82	D_x = 1.372 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2900 reflections
a = 21.746 (6) Å	θ = 3.2–26.2º
b = 12.011 (3) Å	μ = 0.23 mm^{-1}
c = 7.700 (2) Å	T = 294 (2) K
β = 99.472 (5)º	Block, colourless
V = 1983.8 (9) Å^3	0.16 × 0.16 × 0.14 mm
Z = 4	

Data collection

Bruker SMART APEX CCD diffractometer	4047 independent reflections
Radiation source: fine-focus sealed tube	2457 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −27→25
T_{min} = 0.938, T_{max} = 0.969	k = −14→14
10889 measured reflections	l = −9→7

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.043	H-atom parameters constrained
$wR(F^2)$ = 0.111	$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 0.6687P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
4047 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
263 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ 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	0.37851 (3)	0.67006 (8)	0.39409 (12)	0.0980 (3)
O1	0.68083 (8)	0.62360 (17)	0.3371 (3)	0.0733 (6)
O2	0.64129 (6)	0.47384 (13)	0.1858 (2)	0.0493 (4)
O3	0.68737 (7)	0.56737 (15)	−0.0796 (2)	0.0604 (5)
O4	1.00413 (7)	0.13543 (13)	0.31364 (19)	0.0476 (4)
N1	0.90937 (7)	0.26639 (15)	0.1402 (2)	0.0401 (4)
N2	0.96127 (7)	0.23334 (15)	0.0708 (2)	0.0410 (4)
H2	0.9660	0.2559	−0.0322	0.049*
N3	1.14908 (10)	0.0721 (2)	−0.1253 (4)	0.0751 (7)
C1	0.56095 (11)	0.6848 (2)	0.3981 (3)	0.0527 (6)
H1	0.5937	0.7319	0.4420	0.063*
C2	0.50132 (12)	0.7084 (2)	0.4265 (3)	0.0589 (7)
H2A	0.4938	0.7707	0.4914	0.071*
C3	0.45322 (11)	0.6391 (2)	0.3581 (3)	0.0552 (7)
C4	0.46278 (10)	0.5459 (2)	0.2630 (3)	0.0557 (7)
H4	0.4296	0.5002	0.2167	0.067*
C5	0.52281 (10)	0.5215 (2)	0.2373 (3)	0.0481 (6)
H5	0.5302	0.4580	0.1748	0.058*
C6	0.57183 (9)	0.59036 (19)	0.3037 (3)	0.0405 (5)
C7	0.63702 (10)	0.5675 (2)	0.2801 (3)	0.0442 (6)
C8	0.70153 (9)	0.44466 (19)	0.1576 (3)	0.0440 (6)
C9	0.73453 (10)	0.3666 (2)	0.2639 (3)	0.0578 (7)
H9	0.7181	0.3364	0.3577	0.069*
C10	0.79233 (10)	0.3328 (2)	0.2315 (3)	0.0567 (7)
H10	0.8149	0.2798	0.3036	0.068*
C11	0.81639 (9)	0.37765 (19)	0.0923 (3)	0.0396 (5)

C12	0.78249 (9)	0.45669 (18)	−0.0154 (3)	0.0407 (5)
H12	0.7987	0.4866	−0.1097	0.049*
C13	0.72453 (9)	0.49122 (19)	0.0170 (3)	0.0413 (5)
C14	0.70980 (14)	0.6149 (3)	−0.2264 (4)	0.0845 (10)
H14A	0.7477	0.6548	−0.1863	0.127*
H14B	0.6791	0.6651	−0.2865	0.127*
H14C	0.7177	0.5568	−0.3055	0.127*
C15	0.87629 (9)	0.33998 (18)	0.0491 (3)	0.0390 (5)
H15	0.8905	0.3708	−0.0477	0.047*
C16	1.00436 (9)	0.16643 (18)	0.1624 (3)	0.0387 (5)
C17	1.05475 (9)	0.13263 (18)	0.0612 (3)	0.0407 (5)
C18	1.11589 (10)	0.1288 (2)	0.1437 (4)	0.0613 (7)
H18	1.1266	0.1456	0.2627	0.074*
C19	1.16111 (12)	0.0994 (3)	0.0448 (5)	0.0795 (9)
H19	1.2024	0.0985	0.1006	0.095*
C20	1.08999 (12)	0.0745 (2)	−0.2004 (4)	0.0613 (7)
H20	1.0804	0.0555	−0.3189	0.074*
C21	1.04152 (10)	0.10353 (19)	−0.1141 (3)	0.0472 (6)
H21	1.0006	0.1034	−0.1733	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0569 (4)	0.1276 (7)	0.1220 (7)	0.0410 (5)	0.0513 (5)	0.0189 (6)
O1	0.0400 (9)	0.0843 (14)	0.0974 (15)	−0.0070 (9)	0.0166 (10)	−0.0315 (12)
O2	0.0293 (7)	0.0608 (11)	0.0622 (10)	0.0054 (7)	0.0206 (7)	−0.0098 (9)
O3	0.0457 (9)	0.0760 (12)	0.0637 (11)	0.0246 (9)	0.0210 (8)	0.0184 (9)
O4	0.0464 (9)	0.0593 (10)	0.0398 (9)	0.0102 (8)	0.0145 (7)	0.0067 (8)
N1	0.0286 (9)	0.0563 (12)	0.0387 (10)	0.0085 (8)	0.0152 (8)	−0.0018 (9)
N2	0.0327 (9)	0.0600 (12)	0.0347 (10)	0.0126 (8)	0.0181 (8)	0.0042 (9)
N3	0.0526 (14)	0.0872 (18)	0.095 (2)	0.0181 (12)	0.0398 (14)	−0.0006 (15)
C1	0.0491 (13)	0.0569 (16)	0.0538 (15)	0.0057 (12)	0.0134 (12)	−0.0055 (12)
C2	0.0636 (16)	0.0619 (17)	0.0565 (16)	0.0238 (14)	0.0255 (14)	0.0012 (13)
C3	0.0401 (13)	0.0753 (18)	0.0558 (16)	0.0239 (13)	0.0250 (12)	0.0166 (14)
C4	0.0349 (12)	0.0714 (18)	0.0634 (17)	0.0033 (12)	0.0155 (11)	0.0032 (14)
C5	0.0397 (12)	0.0547 (15)	0.0530 (14)	0.0055 (11)	0.0166 (11)	−0.0040 (12)
C6	0.0340 (11)	0.0504 (14)	0.0397 (12)	0.0087 (10)	0.0137 (9)	0.0036 (11)
C7	0.0363 (12)	0.0549 (15)	0.0433 (13)	0.0027 (11)	0.0122 (10)	0.0000 (12)
C8	0.0263 (10)	0.0564 (15)	0.0533 (14)	0.0044 (10)	0.0180 (10)	−0.0032 (12)
C9	0.0440 (13)	0.0779 (18)	0.0588 (16)	0.0128 (13)	0.0297 (12)	0.0178 (14)
C10	0.0409 (12)	0.0773 (18)	0.0569 (15)	0.0208 (12)	0.0233 (11)	0.0211 (14)
C11	0.0277 (10)	0.0522 (14)	0.0410 (12)	0.0061 (10)	0.0118 (9)	−0.0009 (11)
C12	0.0328 (11)	0.0508 (14)	0.0425 (13)	0.0022 (10)	0.0174 (10)	0.0017 (11)
C13	0.0316 (11)	0.0481 (14)	0.0455 (13)	0.0074 (10)	0.0098 (10)	0.0008 (11)
C14	0.079 (2)	0.098 (2)	0.084 (2)	0.0399 (18)	0.0359 (17)	0.0445 (19)
C15	0.0307 (10)	0.0513 (14)	0.0378 (12)	0.0022 (10)	0.0141 (9)	−0.0001 (11)
C16	0.0313 (10)	0.0463 (13)	0.0407 (13)	0.0033 (10)	0.0127 (9)	−0.0002 (11)
C17	0.0334 (11)	0.0440 (13)	0.0479 (14)	0.0080 (9)	0.0156 (10)	0.0060 (11)

C18	0.0390 (13)	0.0826 (19)	0.0621 (17)	0.0163 (13)	0.0079 (12)	0.0034 (15)
C19	0.0325 (13)	0.102 (2)	0.106 (3)	0.0201 (14)	0.0184 (15)	0.004 (2)
C20	0.0636 (17)	0.0648 (18)	0.0632 (17)	0.0102 (14)	0.0331 (14)	−0.0056 (14)
C21	0.0420 (12)	0.0512 (14)	0.0523 (15)	0.0075 (11)	0.0195 (11)	−0.0009 (12)

Geometric parameters (Å, °)

Cl1—C3	1.733 (2)	C8—C9	1.368 (3)
O1—C7	1.190 (3)	C8—C13	1.383 (3)
O2—C7	1.351 (3)	C9—C10	1.382 (3)
O2—C8	1.407 (2)	C9—H9	0.9300
O3—C13	1.358 (3)	C10—C11	1.377 (3)
O3—C14	1.422 (3)	C10—H10	0.9300
O4—C16	1.223 (2)	C11—C12	1.390 (3)
N1—C15	1.275 (3)	C11—C15	1.468 (3)
N1—N2	1.384 (2)	C12—C13	1.388 (3)
N2—C16	1.343 (3)	C12—H12	0.9300
N2—H2	0.8600	C14—H14A	0.9600
N3—C20	1.320 (3)	C14—H14B	0.9600
N3—C19	1.334 (4)	C14—H14C	0.9600
C1—C2	1.379 (3)	C15—H15	0.9300
C1—C6	1.388 (3)	C16—C17	1.501 (3)
C1—H1	0.9300	C17—C18	1.377 (3)
C2—C3	1.372 (4)	C17—C21	1.378 (3)
C2—H2A	0.9300	C18—C19	1.385 (3)
C3—C4	1.371 (3)	C18—H18	0.9300
C4—C5	1.383 (3)	C19—H19	0.9300
C4—H4	0.9300	C20—C21	1.380 (3)
C5—C6	1.379 (3)	C20—H20	0.9300
C5—H5	0.9300	C21—H21	0.9300
C6—C7	1.484 (3)		
C7—O2—C8	116.01 (17)	C10—C11—C12	119.98 (18)
C13—O3—C14	117.02 (17)	C10—C11—C15	121.4 (2)
C15—N1—N2	114.13 (16)	C12—C11—C15	118.58 (18)
C16—N2—N1	120.79 (17)	C13—C12—C11	120.33 (19)
C16—N2—H2	119.6	C13—C12—H12	119.8
N1—N2—H2	119.6	C11—C12—H12	119.8
C20—N3—C19	116.4 (2)	O3—C13—C8	116.20 (17)
C2—C1—C6	119.8 (2)	O3—C13—C12	125.38 (19)
C2—C1—H1	120.1	C8—C13—C12	118.4 (2)
C6—C1—H1	120.1	O3—C14—H14A	109.5
C3—C2—C1	119.5 (2)	O3—C14—H14B	109.5
C3—C2—H2A	120.3	H14A—C14—H14B	109.5
C1—C2—H2A	120.3	O3—C14—H14C	109.5
C4—C3—C2	121.8 (2)	H14A—C14—H14C	109.5
C4—C3—Cl1	119.3 (2)	H14B—C14—H14C	109.5
C2—C3—Cl1	118.9 (2)	N1—C15—C11	122.04 (18)
C3—C4—C5	118.6 (2)	N1—C15—H15	119.0
C3—C4—H4	120.7	C11—C15—H15	119.0

C5—C4—H4	120.7	O4—C16—N2	124.75 (17)
C6—C5—C4	120.6 (2)	O4—C16—C17	121.97 (19)
C6—C5—H5	119.7	N2—C16—C17	113.27 (18)
C4—C5—H5	119.7	C18—C17—C21	118.3 (2)
C5—C6—C1	119.73 (19)	C18—C17—C16	120.1 (2)
C5—C6—C7	122.7 (2)	C21—C17—C16	121.62 (19)
C1—C6—C7	117.6 (2)	C17—C18—C19	118.3 (3)
O1—C7—O2	123.2 (2)	C17—C18—H18	120.8
O1—C7—C6	125.0 (2)	C19—C18—H18	120.8
O2—C7—C6	111.79 (19)	N3—C19—C18	124.1 (3)
C9—C8—C13	121.59 (18)	N3—C19—H19	118.0
C9—C8—O2	119.25 (19)	C18—C19—H19	118.0
C13—C8—O2	119.07 (19)	N3—C20—C21	124.1 (3)
C8—C9—C10	119.8 (2)	N3—C20—H20	118.0
C8—C9—H9	120.1	C21—C20—H20	118.0
C10—C9—H9	120.1	C17—C21—C20	118.9 (2)
C11—C10—C9	119.9 (2)	C17—C21—H21	120.6
C11—C10—H10	120.1	C20—C21—H21	120.6
C9—C10—H10	120.1		
C15—N1—N2—C16	172.0 (2)	C14—O3—C13—C8	−179.0 (2)
C6—C1—C2—C3	−1.2 (4)	C14—O3—C13—C12	0.4 (4)
C1—C2—C3—C4	0.5 (4)	C9—C8—C13—O3	179.6 (2)
C1—C2—C3—Cl1	−179.74 (19)	O2—C8—C13—O3	3.2 (3)
C2—C3—C4—C5	0.5 (4)	C9—C8—C13—C12	0.2 (3)
Cl1—C3—C4—C5	−179.16 (18)	O2—C8—C13—C12	−176.2 (2)
C3—C4—C5—C6	−1.0 (4)	C11—C12—C13—O3	−179.8 (2)
C4—C5—C6—C1	0.4 (3)	C11—C12—C13—C8	−0.4 (3)
C4—C5—C6—C7	179.8 (2)	N2—N1—C15—C11	174.10 (19)
C2—C1—C6—C5	0.7 (3)	C10—C11—C15—N1	−1.7 (3)
C2—C1—C6—C7	−178.7 (2)	C12—C11—C15—N1	−178.8 (2)
C8—O2—C7—O1	0.2 (3)	N1—N2—C16—O4	−4.8 (3)
C8—O2—C7—C6	−179.50 (18)	N1—N2—C16—C17	175.74 (18)
C5—C6—C7—O1	−178.8 (2)	O4—C16—C17—C18	−40.3 (3)
C1—C6—C7—O1	0.5 (4)	N2—C16—C17—C18	139.2 (2)
C5—C6—C7—O2	0.8 (3)	O4—C16—C17—C21	138.9 (2)
C1—C6—C7—O2	−179.79 (19)	N2—C16—C17—C21	−41.6 (3)
C7—O2—C8—C9	98.1 (3)	C21—C17—C18—C19	2.0 (4)
C7—O2—C8—C13	−85.4 (3)	C16—C17—C18—C19	−178.8 (2)
C13—C8—C9—C10	0.0 (4)	C20—N3—C19—C18	0.2 (5)
O2—C8—C9—C10	176.5 (2)	C17—C18—C19—N3	−1.4 (5)
C8—C9—C10—C11	−0.1 (4)	C19—N3—C20—C21	0.3 (4)
C9—C10—C11—C12	−0.1 (4)	C18—C17—C21—C20	−1.5 (3)
C9—C10—C11—C15	−177.1 (2)	C16—C17—C21—C20	179.2 (2)
C10—C11—C12—C13	0.3 (3)	N3—C20—C21—C17	0.4 (4)
C15—C11—C12—C13	177.5 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N2—H2···O4^{i}	0.86	2.03	2.807 (2)	150
C19—H19···O1^{ii}	0.93	2.52	3.420 (3)	162

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

Fig. 1

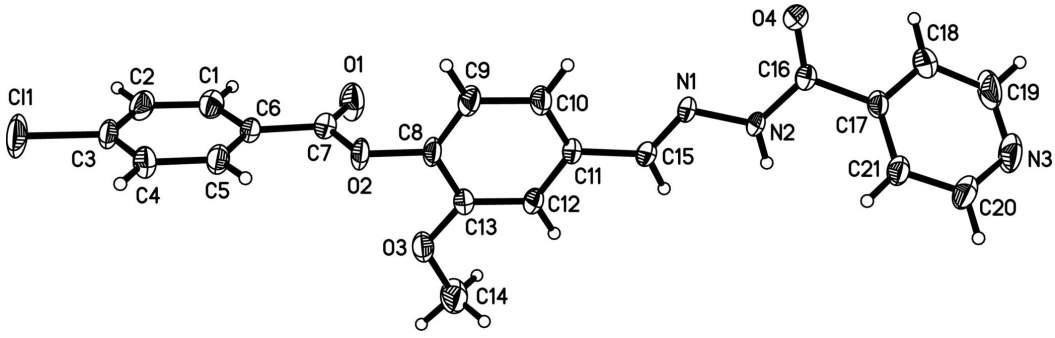
O4
C18
O1
C9
N1
C16
C19
Cl1
C2
C1
C10
C6
C8
N2
C17
C7
C15
N3
C3
C11
C21
O2
C12
C4
C5
C13
C20
O3
C14

Fig. 2