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3-(3-Chlorophenyl)-1-(2-methylimidazo-[1,2-*a*]pyridin-3-yl)prop-2-en-1-one

Yvon Bibila Mayaya Bisseyou,[a]* Adama P. Soro,[a] Drissa Sissouma,[b] Michel Giorgi[c] and N'dédé Ebby[a]

[a]Laboratoire de Cristallographie et Physique Moléculaire, UFR SSMT Université de Cocody, 22 BP 582 Abidjan 22, Cote d'Ivoire, [b]Laboratoire de Chimie Organique Structurale, UFR SSMT Université de Cocody, 22 BP 582 Abidjan 22, Cote d'Ivoire, and [c]Spectropôle Service, Faculté des Sciences et techniques de Saint Jérôme, Avenue Escadrille Normandie Niemen 13397 Marseille, Cedex 20, France
Correspondence e-mail: bibilamayayabisseyou@yahoo.fr

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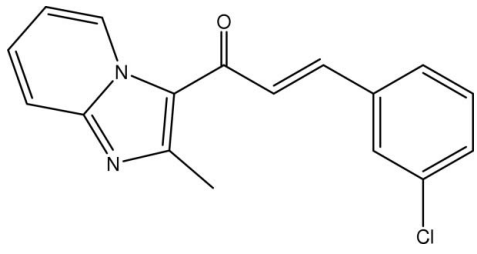
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.091; data-to-parameter ratio = 13.7.

The title compound, $C_{17}H_{13}ClN_2O$, was synthesized from 1-(2-methylimidazo[1,2-*a*]pyridin-3-yl)ethanone and 3-chlorobenzaldehyde in ethanol. The dihedral angle between the imidazopyridine ring system and the benzene ring is 7.43 (1)°. In the solid state, molecules form centrosymmetric $R_2^2(14)$ dimeric units *via* a non-classical C—H···O hydrogen bond. These dimers are arranged in zigzag fashion along the [010] direction.

Related literature

For related crystal structures, see: Zhang and Hu (2005); Duan *et al.* (2006). For properties of chalcones, see: Dimmock *et al.*(1999); Opletalova & Sedivy (1999); Lawrence *et al.* (2001); Mukherjee *et al.* (2001); Lin *et al.* (2002); Bruneton, (1999); Goto *et al.*, (1991); Sarojini *et al.* (2006). For properties of imidazo[1,2-*a*]pyridine derivatives, see: Trapani *et al.* (2003); Gueiffier *et al.* (1998); Mavel *et al.* (2002); Casacchia *et al.*(1989); Morton & Lader (1992); Depoortere *et al.* (1986). For related literature, see: Allen *et al.* (1987); Bernstein *et al.* (1995); Giordanella (2006). For the refinement weighting scheme, see: Watkin (1994); Prince (1982).



Experimental

Crystal data

$C_{17}H_{13}ClN_2O$
M_r = 296.76
Monoclinic, $P2_1/n$
a = 4.784 (2) Å
b = 21.690 (2) Å
c = 13.773 (9) Å
β = 93.425 (4)°
V = 1426.6 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 295 K
0.55 × 0.50 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan *DENZO/SCALEPACK* (Otwinowski & Minor, 1997)
T_{min} = 0.90, T_{max} = 0.95
9741 measured reflections
2608 independent reflections
2076 reflections with $I > 2.0\sigma(I)$
R_{int} = 0.05

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.091
S = 0.88
2608 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{i}	0.95	2.52	3.339 (4)	145

Symmetry code: (i) $-x+2, -y+1, -z+1$.

Data collection: *COLLECT* (Nonius, 1997); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *CRYSTALS*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2207).

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supplementary materials

Acta Cryst. (2007). E**63**, o4758-o4759 [**doi:10.1107/S1600536807050404**]

3-(3-Chlorophenyl)-1-(2-methylimidazo[1,2-*a*]pyridin-3-yl)prop-2-en-1-one

Y. Bibila Mayaya Bisseyou, A. P. Soro, D. Sissouma, M. Giorgi and N. Ebby

Comment

Chalcones and their derivatives and imidazo[1,2-*a*]pyridine derivatives represent two important classes of compound in chemistry, biochemistry and pharmacology. They are the focus of increasing attention because of their potential bioactive profile.

Chalcones and their derivatives have been found to have beneficial biological properties such as anti-inflammatory, anticancer, antibacterial, antiviral, antiprotozoal, antifungal, antiherpes, antitubercular, anti-invasive activities and cytotoxicity, insecticidal, enzyme inhibitory properties (Dimmock *et al.*, 1999; Opletalova & Sedivy, 1999; Lawrence *et al.*, 2001; Mukherjee *et al.*, 2001; Lin *et al.*, 2002). They are also used as intermediates in the synthesis of flavonocols (Bruneton, 1999). Furthermore, it has been reported that several chalcone derivatives present non-linear optical (NLO) properties (Goto *et al.*, 1991; Sarojini *et al.*, 2006).

As for imidazo[1,2-*a*]pyridine derivatives, they are important intermediates in the organic synthesis of therapeutic agents including anticonvulsant (Trapani *et al.*, 2003) and antiviral (Gueiffier *et al.*, 1998; Mavel *et al.*, 2002) agents and are also used in clinical application as anxiolytics and hypnotics (Casacchia *et al.*, 1989; Morton and Lader, 1992; Depoortere *et al.*, 1986). For example, Zolpidem which contains the imidazo[1,2-*a*]pyridine ring system and better known as Stilnox® is the hypnosedative most prescribed in France (Giordanella, 2006). It is well known that while modifying the subtituents around the imidazopyridine nucleus, it is possible to obtain molecules having considerable biological properties. The title compound, highly functionalized, is a chalcone including an imidazo[1,2-*a*]pyridine ring system. This has been synthesized during a research project aimed at searching for new potential therapeutic uses of chalcones and eventually to improve their known properties.

The molecular structure of the title compound and its atomic numbering scheme are illustrated in Fig. 1. The values of bond lengths and angles in the molecule are comparable to those obtained in recent studies of imidazo[1,2-*a*]pyridine derivatives (Zhang and Hu, 2005; Duan *et al.*, 2006). The imidazopyridine ring system is essentially planar, as usually observed, with a maximum deviation of 0.0095 (2) Å for atom C15. This ring system and the benzene ring form a dihedral angle of 7.43 (1)°. The ketone group (C7/C8/C9/O1) is almost planar, with a maximum deviation of 0.0392 (2) Å for C9 from the mean plane. In the benzene ring, bond lengths and angles are within normal ranges (Allen *et al.*,1987). In the three-dimensional crystal packing, carbon atom C5 in molecule at (*x*,*y*,*z*) acts as a hydrogen-bond donor *via* H5 to carbonyl atom O1 in the molecule at (−*x* + 2,-*y* + 1,-*z* + 1), thus forming a centrosymmetric $R^2_2(14)$ (Bernstein *et al.*, 1995) dimeric unit (Fig. 2). These centrosymmetric $R^2_2(14)$ dimers are arranged in zigzag fashion along the [010] direction (Fig. 3).

Experimental

10 ml of NaOH (20%) were added to a cold solution of ethanol (20 ml) and 1-(2-methylimidazo[1,2-*a*]pyridin-3-yl) ethanone (1 g, 5.8 mmol). After 5 minutes of cold agitation, 3-chlorobenzaldehyde (7 mmol) were added in small quantities. The

mixture was stirred at ambient temperature for 3 h. 100 ml of water were added to this suspension. The resulting mixture was neutralized with acetic acid (20%). The precipitate was then filtered, washed many times with water, dried and recrystallized from a mixture of hexane/DCM (3:1). Yellow acicular single crystals of the title compound were obtained for X-ray diffraction analysis (yield: 75%; m.p.: 457 K).

^{1}H (DMSO-d$_6$) δ:2.83 (s, 3H); 7.20 (t, 1H, arom); 7.50 (m, 2H, H vinyl + Harom.); 7.65 (m, 2H, H vinyl + Harom.); 7.80 (m, 2H, H arom.); 7.90 (m, 2H, H arom.); 9.70 (d, 1H, H arom.). ^{13}C (DMSO-d$_6$) δ:18.10 (C, CH3); 110 (C arom.); 118 (2 C arom.); 120 (C arom.); 124 (C arom.); 126 (C vinyl); 128 (2 C arom.); 130 (2 C arom.); 135 (C—Cl); 138 (C arom.); 140 (C arom.); 146 (C vinyl); 152 (C arom.); 179 (C=O). TOF+, SM: 296; m/*z*(%): *M*+1= 297 (35), 296 (100), 268 (47), 185 (77), 132 (53), 90 (38), 78 (58), 51 (42).

Refinement

The H atoms were all located in a difference Fourier map. They were all initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H in the range 0.93–0.99Å and U_{iso}(H) in the range 1.2–1.5 times U_{eq} of the parent atom), after which their positions were refined with riding constraints.

Figures

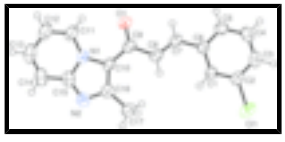

Fig. 1. The molecular structure of the title compound and the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius.

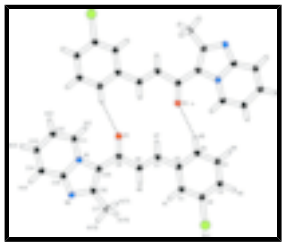

Fig. 2. Part of the crystal structure, showing the formation of a centrosymmetric $R^2_2(14)$ dimer. For the sake of clarity, the unit-cell outline has omitted. Dashed lines indicate C—H···O hydrogen bonds. Atom O1a belongs to the molecule at symmetry position (−*x* + 2,-*y* + 1,-*z* + 1).

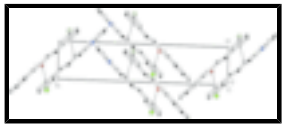

Fig. 3. Crystal packing of the title compound, viewed down the *c* axis, showing centrosymmetric $R^2_2(14)$ dimers arranged in a zigzag fashion along the *b* axis. H atoms not involved in hydrogen bonds have been omitted for clarity. Dashed lines indicate C—H···O hydrogen bonds.

3-(3-Chlorophenyl)-1-(2-methylimidazo[1,2-*a*]pyridin-3-yl)prop-2-en-1-one

Crystal data

$C_{17}H_{13}Cl_1N_2O_1$	F_{000} = 616
M_r = 296.76	D_x = 1.382 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 457 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71070 Å
a = 4.784 (2) Å	Cell parameters from 9741 reflections

b = 21.690 (2) Å	θ = 1.8–26.0º
c = 13.773 (9) Å	μ = 0.27 mm^{-1}
β = 93.425 (4)º	T = 295 K
V = 1426.6 (11) Å^3	Needle, yellow
Z = 4	0.55 × 0.50 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer	2076 reflections with $I > 2.0\sigma(I)$
Monochromator: graphite	R_{int} = 0.05
T = 295 K	θ_{max} = 26.0º
φ scans	θ_{min} = 1.8º
Absorption correction: multi-scan DENZO/SCALEPACK (Otwinowski & Minor, 1997)	$h = -5 \rightarrow 5$
T_{min} = 0.90, T_{max} = 0.95	$k = -24 \rightarrow 26$
9741 measured reflections	$l = -16 \rightarrow 16$
2608 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.047	Method, part 1, Chebychev polynomial, (Watkin, 1994, *P*rince, 1982) [*w*eight] = 1.0/[A_0*T_0(x) + A_1*T_1(x) ··· + A_{n-1}]*T_{n-1}(x)] where A_i are the Chebychev coefficients listed below and x = *F* /*F*max Method = Robust Weighting (*P*rince, 1982) W = [*w*eight] * [1-(delta*F*/6*sigma*F*)^2]^2 A_i are: 211. 268. 175. 53.2
$wR(F^2)$ = 0.091	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.88	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
2608 reflections	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
190 parameters	Extinction correction: None
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.77966 (16)	0.56077 (4)	0.06407 (5)	0.0783
O1	0.8443 (4)	0.40641 (8)	0.44145 (11)	0.0596
N1	0.5302 (4)	0.31509 (7)	0.33536 (12)	0.0418
N2	0.4943 (4)	0.29997 (8)	0.17382 (13)	0.0512
C1	1.4942 (4)	0.52402 (9)	0.21641 (14)	0.0415
C2	1.6944 (4)	0.56347 (10)	0.18489 (15)	0.0442
C3	1.8321 (5)	0.60495 (10)	0.24604 (17)	0.0527
C4	1.7694 (5)	0.60653 (11)	0.34198 (18)	0.0554

C5	1.5692 (5)	0.56696 (10)	0.37618 (16)	0.0488
C6	1.4298 (4)	0.52513 (9)	0.31395 (14)	0.0381
C7	1.2198 (4)	0.48419 (10)	0.35239 (14)	0.0419
C8	1.0923 (4)	0.43741 (9)	0.30706 (14)	0.0428
C9	0.8804 (4)	0.40006 (9)	0.35401 (14)	0.0417
C10	0.7160 (4)	0.35647 (9)	0.29491 (14)	0.0387
C11	0.4667 (5)	0.30482 (10)	0.43006 (17)	0.0554
C12	0.2703 (6)	0.26144 (11)	0.4480 (2)	0.0666
C13	0.1361 (6)	0.22782 (11)	0.3726 (2)	0.0668
C14	0.1991 (5)	0.23756 (10)	0.2791 (2)	0.0591
C15	0.4012 (5)	0.28214 (9)	0.25937 (17)	0.0475
C16	0.6838 (4)	0.34500 (9)	0.19497 (15)	0.0434
C17	0.8231 (5)	0.37501 (11)	0.11281 (15)	0.0549
H5	1.5256	0.5682	0.4424	0.0574*
H8	1.1478	0.4266	0.2439	0.0522*
H4	1.8610	0.6348	0.3850	0.0640*
H7	1.1715	0.4923	0.4162	0.0505*
H1	1.4001	0.4976	0.1730	0.0487*
H14	0.1088	0.2156	0.2262	0.0709*
H3	1.9803	0.6298	0.2218	0.0636*
H11	0.5623	0.3271	0.4800	0.0676*
H12	0.2278	0.2543	0.5120	0.0808*
H13	−0.0031	0.1991	0.3867	0.0814*
H171	0.8229	0.4197	0.1193	0.0802*
H172	0.7273	0.3636	0.0530	0.0805*
H173	1.0211	0.3612	0.1109	0.0818*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0880 (5)	0.0987 (6)	0.0507 (4)	−0.0175 (4)	0.0246 (3)	0.0127 (3)
O1	0.0692 (12)	0.0695 (11)	0.0415 (8)	−0.0186 (8)	0.0148 (7)	−0.0005 (7)
N1	0.0425 (10)	0.0342 (8)	0.0500 (10)	0.0049 (7)	0.0135 (7)	0.0046 (7)
N2	0.0505 (12)	0.0480 (10)	0.0550 (11)	−0.0002 (8)	0.0029 (8)	−0.0014 (8)
C1	0.0365 (12)	0.0463 (11)	0.0419 (10)	−0.0009 (8)	0.0035 (8)	0.0004 (9)
C2	0.0404 (13)	0.0486 (12)	0.0444 (11)	0.0015 (9)	0.0078 (9)	0.0082 (9)
C3	0.0430 (14)	0.0449 (12)	0.0708 (15)	−0.0053 (10)	0.0074 (11)	0.0078 (11)
C4	0.0532 (15)	0.0464 (13)	0.0664 (15)	−0.0071 (10)	0.0008 (11)	−0.0095 (11)
C5	0.0508 (14)	0.0510 (12)	0.0449 (11)	0.0015 (10)	0.0061 (9)	−0.0057 (9)
C6	0.0331 (11)	0.0414 (10)	0.0400 (10)	0.0036 (8)	0.0039 (8)	0.0020 (8)
C7	0.0395 (12)	0.0496 (12)	0.0376 (10)	0.0040 (9)	0.0094 (8)	0.0032 (9)
C8	0.0405 (12)	0.0474 (11)	0.0414 (10)	0.0013 (9)	0.0106 (8)	0.0012 (9)
C9	0.0407 (13)	0.0423 (11)	0.0428 (11)	0.0050 (9)	0.0094 (8)	0.0040 (8)
C10	0.0388 (12)	0.0357 (10)	0.0426 (10)	0.0037 (8)	0.0118 (8)	0.0035 (8)
C11	0.0688 (16)	0.0437 (12)	0.0561 (13)	−0.0014 (11)	0.0243 (11)	0.0063 (10)
C12	0.080 (2)	0.0451 (13)	0.0779 (17)	−0.0036 (12)	0.0345 (14)	0.0106 (12)
C13	0.0590 (17)	0.0384 (12)	0.106 (2)	−0.0038 (11)	0.0255 (15)	0.0096 (13)
C14	0.0498 (15)	0.0388 (12)	0.0890 (18)	0.0002 (10)	0.0063 (12)	0.0028 (12)

C15	0.0424 (13)	0.0356 (11)	0.0650 (14)	0.0047 (9)	0.0058 (10)	0.0012 (10)
C16	0.0417 (12)	0.0410 (11)	0.0479 (11)	0.0072 (9)	0.0064 (8)	0.0021 (9)
C17	0.0624 (16)	0.0618 (14)	0.0413 (12)	−0.0014 (11)	0.0091 (10)	0.0040 (10)

Geometric parameters (Å, °)

Cl1—C2	1.738 (2)	C7—C8	1.321 (3)
O1—C9	1.234 (2)	C7—H7	0.939
N1—C10	1.402 (2)	C8—C9	1.477 (3)
N1—C11	1.375 (3)	C8—H8	0.954
N1—C15	1.382 (3)	C9—C10	1.448 (3)
N2—C15	1.341 (3)	C10—C16	1.398 (3)
N2—C16	1.353 (3)	C11—C12	1.363 (3)
C1—C2	1.374 (3)	C11—H11	0.936
C1—C6	1.396 (3)	C12—C13	1.394 (4)
C1—H1	0.926	C12—H12	0.930
C2—C3	1.373 (3)	C13—C14	1.355 (4)
C3—C4	1.373 (3)	C13—H13	0.941
C3—H3	0.967	C14—C15	1.406 (3)
C4—C5	1.389 (3)	C14—H14	0.952
C4—H4	0.942	C16—C17	1.496 (3)
C5—C6	1.391 (3)	C17—H171	0.973
C5—H5	0.948	C17—H172	0.951
C6—C7	1.463 (3)	C17—H173	0.995
C10—N1—C11	131.44 (19)	C8—C9—C10	118.41 (17)
C10—N1—C15	107.16 (17)	O1—C9—C10	121.23 (19)
C11—N1—C15	121.40 (19)	C9—C10—N1	122.03 (17)
C15—N2—C16	105.81 (19)	C9—C10—C16	133.92 (18)
C2—C1—C6	119.42 (19)	N1—C10—C16	104.01 (18)
C2—C1—H1	120.2	N1—C11—C12	118.5 (2)
C6—C1—H1	120.4	N1—C11—H11	119.2
Cl1—C2—C1	119.31 (17)	C12—C11—H11	122.3
Cl1—C2—C3	118.54 (17)	C11—C12—C13	121.2 (2)
C1—C2—C3	122.1 (2)	C11—C12—H12	118.7
C2—C3—C4	118.8 (2)	C13—C12—H12	120.2
C2—C3—H3	119.2	C12—C13—C14	120.5 (2)
C4—C3—H3	121.7	C12—C13—H13	119.5
C3—C4—C5	120.4 (2)	C14—C13—H13	120.0
C3—C4—H4	120.1	C13—C14—C15	119.1 (2)
C5—C4—H4	119.5	C13—C14—H14	122.1
C4—C5—C6	120.6 (2)	C15—C14—H14	118.8
C4—C5—H5	120.2	C14—C15—N1	119.4 (2)
C6—C5—H5	119.2	C14—C15—N2	129.6 (2)
C1—C6—C5	118.62 (19)	N1—C15—N2	111.09 (19)
C1—C6—C7	122.23 (18)	C10—C16—N2	111.93 (18)
C5—C6—C7	119.15 (18)	C10—C16—C17	129.7 (2)
C6—C7—C8	127.05 (18)	N2—C16—C17	118.32 (19)
C6—C7—H7	116.0	C16—C17—H171	111.1
C8—C7—H7	116.9	C16—C17—H172	109.2

C7—C8—C9	121.61 (19)	H171—C17—H172	109.6
C7—C8—H8	118.2	C16—C17—H173	110.9
C9—C8—H8	120.1	H171—C17—H173	108.0
C8—C9—O1	120.4 (2)	H172—C17—H173	108.0

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.95	2.52	3.339 (4)	145

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

Fig. 1

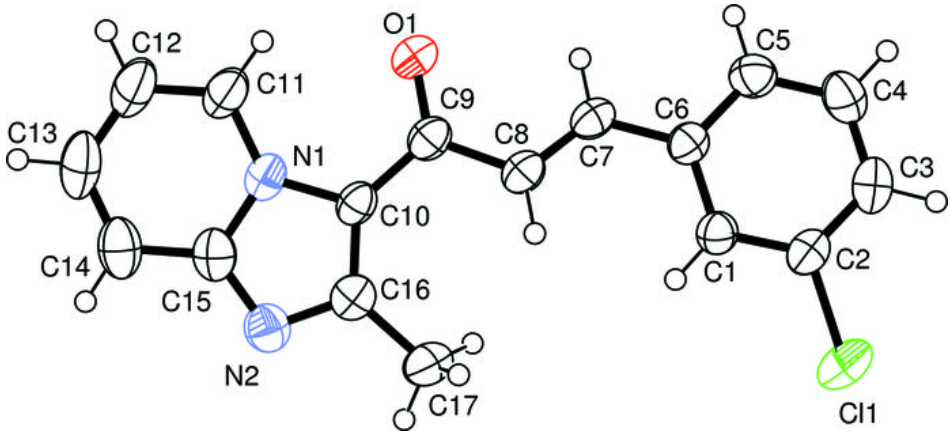
O1
C12
C11
C9
C5
C4
C13
N1
C8
C7
C6
C3
C10
C14
C15
C16
C1
C2
N2
C17
Cl1

Fig. 2

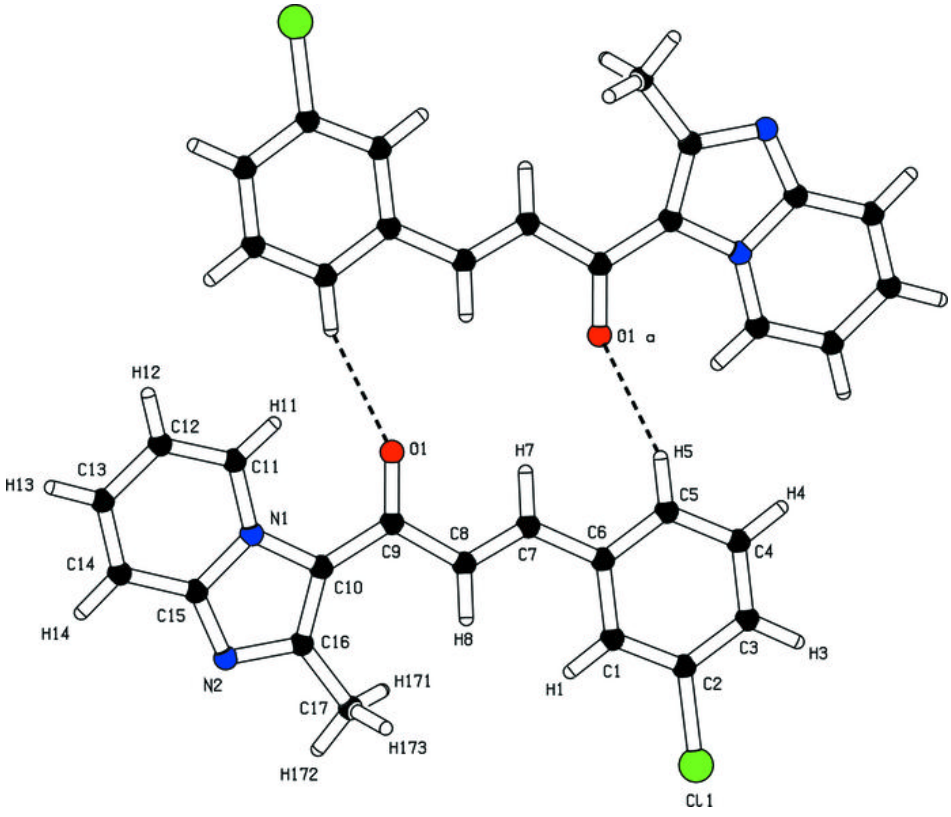
O1 a
H12
H11
C12
C11
O1
H7
H5
C13
H13
C5
H4
N1
C8
C6
C9
C7
C4
C14
C10
C15
H14
H8
C16
C3
H3
N2
C1
H171
C17
C2
H1
H173
H172
CL1

Fig. 3