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(*E*)-2-(2,6-Dichlorophenyl)-2-(phenylimino)acetamide

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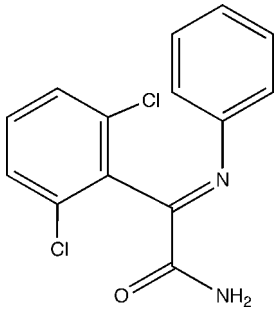
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.135; data-to-parameter ratio = 16.2.

In the title compound, $C_{14}H_{10}Cl_2N_2O$, which is an important synthetic precursor of a human immunodeficiency virus type 1 (HIV-1) inhibitor, the dihedral angle between the 2,6-dichlorophenyl ring and the phenyl ring is 69.4 (1)°. In the crystal structure, the molecules form centrosymmetric dimers *via* N—H···O hydrogen bonds with an $R_2^2(8)$ motif. The dimers are connected by intermolecular C—H···O and C—H···π interactions.

Related literature

For the starting material, see: Reich *et al.* (1917). For human immunodeficiency virus type 1 inhibitors, see: Pauwels *et al.* (1993). For related literature on the crystal structures of α-anilinoacetamide derivatives, see: Peeters *et al.* (1993); Garg *et al.* (1993); Opatz & Ferenc (2005). For related literature on C—H···O hydrogen bonds, see: Taylor & Kennard (1982); Biradha *et al.* (1997); Batchelor *et al.* (2000). For related literature on C—H···π interactions, see: Malone *et al.* (1997); Tomura & Yamashita (2001); Nishio (2004). For related literature, see: Allen *et al.* (1987); Bernstein *et al.* (1995); Allen (2002).



Experimental

Crystal data

$C_{14}H_{10}Cl_2N_2O$
M_r = 293.14
Triclinic, $P\overline{1}$
a = 7.8777 (2) Å
b = 9.1433 (3) Å
c = 10.0217 (4) Å
α = 102.170 (3)°
β = 91.795 (3)°
γ = 102.145 (2)°
V = 687.66 (4) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 4.19 mm^{-1}
T = 296 (1) K
0.50 × 0.40 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.229, T_{max} = 0.818
3020 measured reflections
2808 independent reflections
2499 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
3 standard reflections
frequency: 120 min
intensity decay: 0.8%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.135
S = 1.05
2808 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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}	0.86	2.08	2.935 (2)	172
N2—H2B···N1	0.86	2.37	2.708 (2)	104
C3—H3···O1^{ii}	0.93	2.55	3.260 (2)	133
N2—H2B···$Cg1^{iii}$	0.86	2.76	3.484 (2)	143

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+2$; (iii) $-x, -y, -z+1$. $Cg1$ is the centroid of the C8–C13 benzene ring.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1992); cell refinement: *CAD-4 EXPRESS*; data reduction: *TEXSAN* (Rigaku/MSC, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

The author thanks the Instrument Center of the Institute for Molecular Science for the X-ray structure analysis.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2151).

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supplementary materials

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(*E*)-2-(2,6-Dichlorophenyl)-2-(phenylimino)acetamide

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Comment

The title compound, (I), is an important synthetic precursor of α-anilinophenylaceamide derivatives, which are potent human immunodeficiency virus type 1 (HIV-1) specific reverse transcriptase inhibitors (Pauwels *et al.*, 1993). A search for α-anilinoaceamide structure in the Cambridge Structural Database (Version 5.28; Allen, 2002) revealed three examples (Peeters *et al.*, 1993; Garg *et al.*, 1993; Opatz & Ferenc, 2005) while no structure of an α-phenyliminoaceamide derivative, such as (I), was found. We report here the molecular and crystal structures of the title α-phenyliminoaceamide derivative (I) (Fig. 1).

The compound (I) was synthesized by the reaction of *N*-(2,6-dichlorobenzylidene)aniline (Reich *et al.*, 1917) with NaCN and crystallizes in the $P\bar{1}$ space group with one molecule in an asymmetric unit. The molecule has an *E*-conformation about the C7═N1 bond. The bond lengths and angles are within the normal ranges (Allen *et al.*, 1987). Two benzene rings of (I) are planar [r.m.s. deviations of 0.0047 (C1—C6) and 0.0074 (C8—C13) Å from the least-squares planes] with a dihedral angle between their least-squares planes of 69.4 (1)°. Each benzene ring is close to be orthogonal [86.5 (2) for C1—C6 and 73.9 (1)° for C8—C13] to the plane of the amide group (C14/O1/N2). In the amide group, the intramolecular hydrogen bond between atoms N1 and N2 is observed [2.708 (2) Å].

In the crystal structure, the molecules are linked *via* N—H···O hydrogen bonds [2.935 (2) Å for N2—H2A···O1(−*x* + 1, −*y* + 1, −*z* + 1)] to form a centrosymmetric dimer with a graph-set motif (Bernstein *et al.*, 1995) of $R_2^2(8)$ (Fig. 2 and Table 1). The intermolecular C—H···O [3.260 (2) Å for C3—H3···O1(−*x* + 1, −*y* + 1, −*z* + 2)] and C—H···π [3.484 (2) Å for N2—H2B···*Cg*1(−*x*, −*y*, −*z* + 1), *Cg*1 is the centroid of the benzene ring (C8—C13)] interactions are observed between the dimers (Tomura & Yamashita, 2001; Nishio, 2004). The C—H···O hydrogen bond in the crystal structure of (I) is stronger than the typical C—H···O hydrogen bonds in other structures (Taylor & Kennard, 1982; Biradha *et al.*, 1997; Batchelor *et al.*, 2000). The C—H···π interaction corresponds to a geometry of type III (Malone *et al.*, 1997).

Experimental

The compound (I) was prepared as follows: a mixture of *N*-(2,6-dichlorobenzylidene)aniline (Reich *et al.*, 1917) (504 mg, 2.0 mmol) and NaCN (110 mg, 2.0 mmol) in dimethyl sulfoxide (20 ml) was stirred for 1 day at 296 K. The reaction mixture was poured into water (100 ml) and the solution was extracted with dichloromethane (100 ml × 3). The organic layer was washed with water and dried over Na_2SO_4. After the solvent was evaporated *in vacuo*, dichloromethane (10 ml) was added to the residue. The resulting colourless precipitate was collected to give 198 mg (34% yield) of (I). Physical data for (I): m.p. 510 K; ^{1}H NMR ($CDCl_3$, δ p.p.m.): 5.30–5.65 (br s, 1H), 6.81–7.26 (m, 8H), 7.37–7.47 (br s, 1H); MS (EI): m/*z* 294 (M^++2), 292 (M^+), 248. Colourless crystals of (I) suitable for X-ray analysis were grown from a chloroform solution.

Refinement

All H atoms were placed in geometrically calculated positions and refined using a riding model, with C—H = 0.93 Å, N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C) or (N).

Figures

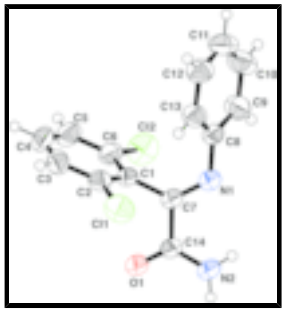

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms and H atoms are shown as small spheres of arbitrary radii.

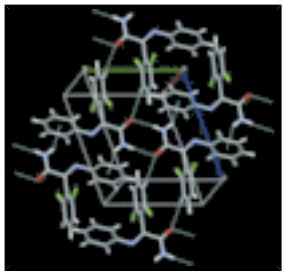

Fig. 2. The packing diagram of (I). Dashed lines indicate intermolecular N—H···O, C—H···O and C—H···π interactions.

(*E*)-2-(2,6-Dichlorophenyl)-2-(phenylimino)acetamide

Crystal data

$C_{14}H_{10}Cl_2N_2O$	$Z = 2$
$M_r = 293.14$	$F_{000} = 300$
Triclinic, $P\overline{1}$	$D_x = 1.416$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 510 K
$a = 7.8777$ (2) Å	Cu $K\alpha$ radiation $\lambda = 1.54178$ Å
$b = 9.1433$ (3) Å	Cell parameters from 25 reflections
$c = 10.0217$ (4) Å	$\theta = 15.0$–42.6^o
$\alpha = 102.170$ (3)º	$\mu = 4.19$ mm^{-1}
$\beta = 91.795$ (3)º	$T = 296$ (1) K
$\gamma = 102.145$ (2)º	Prism, colourless
$V = 687.66$ (4) Å^3	0.50 × 0.40 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.016$

Monochromator: graphite	θ_{max} = 74.3º
T = 296(1) K	θ_{min} = 4.5º
ω–2θ scan	h = 0→9
Absorption correction: ψ scan (North *et al.*, 1968)	k = −11→11
T_{min} = 0.229, T_{max} = 0.818	l = −12→12
3020 measured reflections	3 standard reflections
2808 independent reflections	every 120 min
2499 reflections with $I > 2\sigma(I)$	intensity decay: 0.8%

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$w = 1/[\sigma^2(F_o^2) + (0.0796P)^2 + 0.1897P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.135	$(\Delta/\sigma)_{max} < 0.001$
S = 1.05	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
2808 reflections	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
173 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0156 (17)
Secondary atom site location: difference Fourier map	

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 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	0.15690 (8)	0.38587 (7)	0.87469 (7)	0.0713 (2)
Cl2	0.62681 (8)	0.04600 (8)	0.72009 (7)	0.0791 (2)
O1	0.5291 (2)	0.42558 (17)	0.65152 (14)	0.0632 (4)
N1	0.2306 (2)	0.07483 (17)	0.59095 (15)	0.0472 (4)
N2	0.3232 (2)	0.3200 (2)	0.47621 (16)	0.0598 (5)
H2A	0.3588	0.3906	0.4323	0.072*
H2B	0.2355	0.2462	0.4425	0.072*

C1	0.3973 (2)	0.21737 (18)	0.81031 (16)	0.0413 (4)
C2	0.3294 (2)	0.3076 (2)	0.91479 (18)	0.0476 (4)
C3	0.3924 (3)	0.3366 (3)	1.0501 (2)	0.0611 (6)
H3	0.3451	0.3986	1.1180	0.073*
C4	0.5255 (3)	0.2723 (3)	1.0823 (2)	0.0720 (7)
H4	0.5683	0.2902	1.1732	0.086*
C5	0.5971 (3)	0.1818 (3)	0.9828 (2)	0.0690 (6)
H5	0.6872	0.1382	1.0061	0.083*
C6	0.5340 (3)	0.1557 (2)	0.8470 (2)	0.0515 (4)
C7	0.3324 (2)	0.19374 (19)	0.66374 (16)	0.0412 (4)
C8	0.1608 (2)	−0.0528 (2)	0.64758 (18)	0.0471 (4)
C9	0.1897 (3)	−0.1957 (2)	0.5867 (2)	0.0622 (5)
H9	0.2556	−0.2065	0.5113	0.075*
C10	0.1197 (3)	−0.3220 (3)	0.6390 (3)	0.0724 (7)
H10	0.1420	−0.4171	0.6000	0.087*
C11	0.0181 (3)	−0.3085 (3)	0.7476 (3)	0.0695 (6)
H11	−0.0290	−0.3942	0.7815	0.083*
C12	−0.0139 (3)	−0.1682 (3)	0.8058 (3)	0.0649 (6)
H12	−0.0836	−0.1594	0.8790	0.078*
C13	0.0564 (3)	−0.0396 (2)	0.7570 (2)	0.0541 (5)
H13	0.0340	0.0551	0.7971	0.065*
C14	0.4032 (2)	0.3250 (2)	0.59550 (17)	0.0449 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0733 (4)	0.0624 (4)	0.0828 (4)	0.0283 (3)	0.0142 (3)	0.0118 (3)
Cl2	0.0702 (4)	0.0934 (5)	0.0848 (4)	0.0427 (3)	0.0105 (3)	0.0191 (3)
O1	0.0780 (10)	0.0577 (8)	0.0474 (7)	−0.0110 (7)	−0.0061 (6)	0.0245 (6)
N1	0.0523 (8)	0.0469 (8)	0.0428 (7)	0.0070 (6)	0.0000 (6)	0.0155 (6)
N2	0.0740 (11)	0.0567 (9)	0.0480 (9)	−0.0007 (8)	−0.0090 (8)	0.0272 (7)
C1	0.0463 (9)	0.0404 (8)	0.0378 (8)	0.0021 (7)	0.0029 (6)	0.0173 (6)
C2	0.0520 (10)	0.0424 (9)	0.0467 (9)	0.0018 (7)	0.0090 (7)	0.0140 (7)
C3	0.0704 (13)	0.0610 (12)	0.0400 (9)	−0.0096 (10)	0.0083 (9)	0.0088 (8)
C4	0.0816 (16)	0.0808 (15)	0.0419 (10)	−0.0152 (12)	−0.0111 (10)	0.0235 (10)
C5	0.0646 (13)	0.0763 (14)	0.0678 (14)	0.0035 (11)	−0.0171 (11)	0.0352 (12)
C6	0.0499 (10)	0.0551 (10)	0.0519 (10)	0.0081 (8)	0.0004 (8)	0.0212 (8)
C7	0.0460 (9)	0.0432 (8)	0.0376 (8)	0.0105 (7)	0.0041 (6)	0.0153 (6)
C8	0.0473 (9)	0.0468 (9)	0.0468 (9)	0.0041 (7)	−0.0047 (7)	0.0173 (7)
C9	0.0667 (13)	0.0526 (11)	0.0663 (12)	0.0107 (9)	0.0070 (10)	0.0136 (9)
C10	0.0703 (14)	0.0477 (11)	0.1013 (19)	0.0132 (10)	−0.0044 (13)	0.0231 (11)
C11	0.0565 (12)	0.0630 (13)	0.0950 (17)	0.0009 (10)	−0.0058 (11)	0.0445 (12)
C12	0.0530 (11)	0.0709 (14)	0.0712 (13)	−0.0013 (10)	0.0054 (10)	0.0318 (11)
C13	0.0493 (10)	0.0518 (10)	0.0596 (11)	0.0028 (8)	0.0025 (8)	0.0175 (8)
C14	0.0550 (10)	0.0440 (9)	0.0380 (8)	0.0095 (7)	0.0051 (7)	0.0154 (7)

Geometric parameters (Å, °)

Cl1—C2	1.737 (2)	C4—H4	0.9300

Cl2—C6	1.728 (2)	C5—C6	1.388 (3)
O1—C14	1.228 (2)	C5—H5	0.9300
N1—C7	1.273 (2)	C7—C14	1.519 (2)
N1—C8	1.420 (2)	C8—C13	1.391 (3)
N2—C14	1.322 (2)	C8—C9	1.389 (3)
N2—H2A	0.8600	C9—C10	1.385 (3)
N2—H2B	0.8600	C9—H9	0.9300
C1—C2	1.385 (2)	C10—C11	1.371 (4)
C1—C6	1.389 (3)	C10—H10	0.9300
C1—C7	1.496 (2)	C11—C12	1.371 (4)
C2—C3	1.381 (3)	C11—H11	0.9300
C3—C4	1.367 (4)	C12—C13	1.384 (3)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.372 (4)	C13—H13	0.9300
C7—N1—C8	120.81 (14)	N1—C7—C14	117.73 (14)
C14—N2—H2A	120.0	C1—C7—C14	115.27 (14)
C14—N2—H2B	120.0	C13—C8—C9	119.52 (18)
H2A—N2—H2B	120.0	C13—C8—N1	121.59 (17)
C2—C1—C6	117.04 (16)	C9—C8—N1	118.78 (18)
C2—C1—C7	121.51 (16)	C10—C9—C8	119.5 (2)
C6—C1—C7	121.38 (16)	C10—C9—H9	120.2
C3—C2—C1	122.56 (19)	C8—C9—H9	120.2
C3—C2—Cl1	118.54 (17)	C11—C10—C9	120.8 (2)
C1—C2—Cl1	118.89 (14)	C11—C10—H10	119.6
C4—C3—C2	118.6 (2)	C9—C10—H10	119.6
C4—C3—H3	120.7	C12—C11—C10	119.7 (2)
C2—C3—H3	120.7	C12—C11—H11	120.2
C5—C4—C3	121.14 (19)	C10—C11—H11	120.2
C5—C4—H4	119.4	C11—C12—C13	120.8 (2)
C3—C4—H4	119.4	C11—C12—H12	119.6
C4—C5—C6	119.4 (2)	C13—C12—H12	119.6
C4—C5—H5	120.3	C12—C13—C8	119.6 (2)
C6—C5—H5	120.3	C12—C13—H13	120.2
C1—C6—C5	121.2 (2)	C8—C13—H13	120.2
C1—C6—Cl2	118.90 (14)	O1—C14—N2	124.57 (16)
C5—C6—Cl2	119.94 (18)	O1—C14—C7	119.44 (15)
N1—C7—C1	126.95 (15)	N2—C14—C7	115.98 (16)
C6—C1—C2—C3	−0.1 (3)	C6—C1—C7—N1	79.6 (2)
C7—C1—C2—C3	−177.07 (16)	C2—C1—C7—C14	79.1 (2)
C6—C1—C2—Cl1	−179.37 (13)	C6—C1—C7—C14	−97.79 (19)
C7—C1—C2—Cl1	3.6 (2)	C7—N1—C8—C13	60.6 (3)
C1—C2—C3—C4	−0.7 (3)	C7—N1—C8—C9	−123.2 (2)
Cl1—C2—C3—C4	178.54 (15)	C13—C8—C9—C10	−2.5 (3)
C2—C3—C4—C5	0.6 (3)	N1—C8—C9—C10	−178.79 (19)
C3—C4—C5—C6	0.4 (3)	C8—C9—C10—C11	2.0 (4)
C2—C1—C6—C5	1.1 (3)	C9—C10—C11—C12	−0.5 (4)
C7—C1—C6—C5	178.08 (17)	C10—C11—C12—C13	−0.5 (4)
C2—C1—C6—Cl2	−178.50 (13)	C11—C12—C13—C8	0.0 (3)

C7—C1—C6—Cl2	−1.5 (2)	C9—C8—C13—C12	1.5 (3)
C4—C5—C6—C1	−1.3 (3)	N1—C8—C13—C12	177.73 (18)
C4—C5—C6—Cl2	178.32 (17)	N1—C7—C14—O1	−164.09 (18)
C8—N1—C7—C1	2.0 (3)	C1—C7—C14—O1	13.6 (3)
C8—N1—C7—C14	179.41 (16)	N1—C7—C14—N2	15.0 (3)
C2—C1—C7—N1	−103.5 (2)	C1—C7—C14—N2	−167.32 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O1^{i}	0.86	2.08	2.935 (2)	172
N2—H2B···N1	0.86	2.37	2.708 (2)	104
C3—H3···O1^{ii}	0.93	2.55	3.260 (2)	133
N2—H2B···Cg1^{iii}	0.86	2.76	3.484 (2)	143

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

Fig. 1

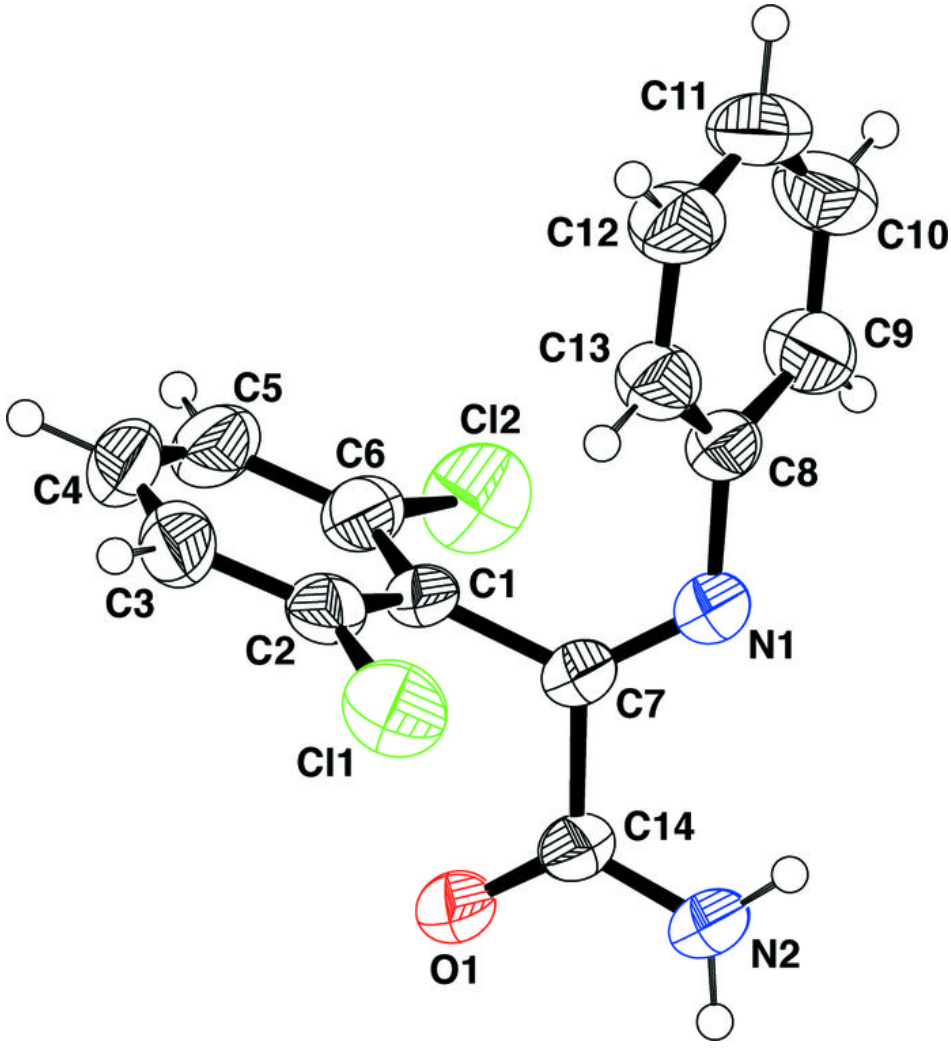

Fig. 2