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N,*N*′-(4,5-Dichloro-*o*-phenylene)-dibenzamide

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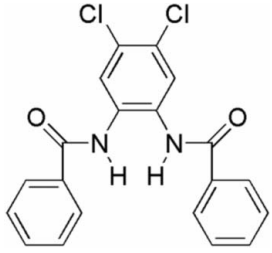
Key indicators: single-crystal X-ray study; T = 288 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.114; data-to-parameter ratio = 14.5.

In the title molecule, $C_{20}H_{14}Cl_2N_2O_2$, the dihedral angles between the central benzene ring and the two outer phenyl rings are 58.92 (7) and 21.91 (9)°. While an intramolecluar N—H···O hydrogen bond may influence the molecular conformation, an intermolecular N—H···O hydrogen bond connects molecules into centrosymetric dimers.

Related literature

For background information, see: Baik *et al.* (2003); Costa *et al.* (2004); Abu-Omar *et al.* (2005); Girerd *et al.* (2000).



Experimental

Crystal data

$C_{20}H_{14}Cl_2N_2O_2$
M_r = 385.23
Monoclinic, $P2_1/c$
a = 8.3024 (8) Å
b = 11.8571 (11) Å
c = 18.7334 (18) Å
β = 102.630 (2)°
V = 1799.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 288 (2) K
0.08 × 0.03 × 0.03 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.986, T_{max} = 0.989
9881 measured reflections
3518 independent reflections
1936 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.114
S = 1.00
3518 reflections
243 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N···O1^{i}	0.85 (3)	2.15 (3)	2.976 (3)	165 (3)
C5—H5···O1	0.93	2.44	2.769 (3)	101
N1—H1N···O2	0.87 (3)	1.93 (3)	2.702 (3)	147 (2)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: LH2410).

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supplementary materials

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N,*N*'-(4,5-Dichloro-*o*-phenylene)dibenzamide

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Comment

Dioxygen is activated by nonheme biological systems to carry out selective transformations of organic substrates (Baik *et al.*, 2003). Key intermediates such as Fe(IV)-oxo and Fe(V)-oxo compounds have been identified or proposed in bleomycin, naphthalene dioxygenase, and Rieske dioxygenase (Costa *et al.*, 2004, Abu-Omar *et al.* 2005). Considerable efforts have been devoted to prepare and characterize models of these intermediates. Amine/pyridine ligands have often been used and have allowed the identification of synthetic models of the intermediates (Costa *et al.*, 2004, Girerd *et al.*, 2000). In order to further develop functional models for mononuclear nonheme iron oxygenases, we synthesized a new N_2–type bidentate ligand.

The asymmetric unit of (I) contains whole molecule in a monoclinic cell (space group P21/c) with $Z = 4$. The molecule is not planar, having large twisted angles between benzene ring (A) and phenyl rings (B and C) (Fig. 1). The dihedral angle between ring A and ring B is 58.92 (7)°, and the dihedral angle between ring A and ring C is 21.91 (9)°. There are intramolecular hydrogen bonds between an amide hydrogen atom and an amide oxygen atom (N1(amide)-H1N···O2(amide) 2.702 (3) A%), and between a phenyl hydrogen atom and amide oxygen atom (C5—H5···O1(amide) 2.769 (3) A%). There are also intermolecular hydrogen bonds between amide hydrogen atoms and amide oxygen atoms of neighboring molecules (N2(amide)-H2N···O1(amide) 2.976 (3) A%) with a N2—H2N···O1 angle of 165 (3)°. These intermolecular hydrogen bonds form a dimeric molecule as shown in Fig. 2.

Experimental

To a stirred solution of 4,5-dichloro-1,2-phenylenediamine (0.92 g, 5 mmol) in THF (100 ml), a solution of triethylamine (2.10 ml, 15 mmol) was added dropwise. The solution was stirred for 15 min and benzoyl chloride (1.17 ml, 10 mmol) was slowly added. The reaction mixture was stirred for 4 h at room temperature. Then, the solution was evaporated to dryness. The powder was collected by filtration, washed with MeOH, and dried under vacuum oven for 1 h. Recrystallization from a methanol solution afforded an ivory powder. Colorless rod-type crystals were prepared from a DMSO-acetone solution at room temperature by slow evaporation for X-ray experiments.

Refinement

H atoms were placed in calculated positions with C—H distances of 0.93 Å·They were included in the refinement in riding–motion approximation with $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms bonded to N atoms were refined independently with isotropic displacement parameters

Figures

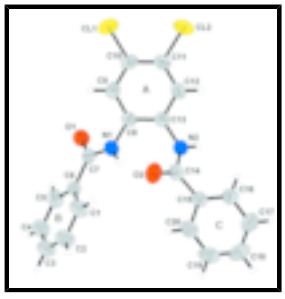

Fig. 1. The molecluar structure of the title compound showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

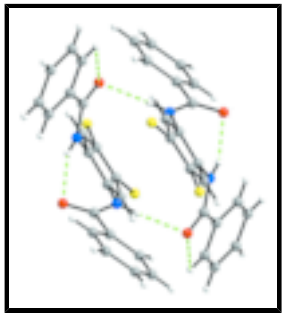

Fig. 2. A hydrogen-bonded dimer of the title compound showing hydrogen bonds as dashed lines.

N,*N*'-(4,5-Dichloro-*o*-phenylene)dibenzamide

Crystal data

$C_{20}H_{14}Cl_2N_2O_2$	F_{000} = 792
M_r = 385.23	D_x = 1.422 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 986 reflections
a = 8.3024 (8) Å	θ = 2.2–18.8º
b = 11.8571 (11) Å	μ = 0.38 mm^{-1}
c = 18.7334 (18) Å	T = 288 (2) K
β = 102.630 (2)º	Rod, colorless
V = 1799.5 (3) Å^3	0.08 × 0.03 × 0.03 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	3518 independent reflections
Radiation source: fine-focus sealed tube	1936 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.048
T = 288(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −10→9
T_{min} = 0.986, T_{max} = 0.989	k = −14→14

9881 measured reflections

$l = -19 \rightarrow 23$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.114$

$S = 1.00$

3518 reflections

243 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2 + 0.2774P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.16$ e Å^{-3}

$\Delta\rho_{min} = -0.19$ e Å^{-3}

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	0.28862 (10)	1.37684 (6)	1.07001 (5)	0.0748 (3)
Cl2	0.00258 (11)	1.37867 (6)	0.92701 (5)	0.0839 (3)
N1	0.3210 (3)	0.95030 (19)	1.04178 (14)	0.0450 (6)
H1N	0.345 (3)	0.906 (2)	1.0091 (15)	0.047 (8)*
N2	0.0736 (3)	0.95613 (18)	0.90593 (12)	0.0415 (6)
H2N	−0.029 (4)	0.962 (2)	0.8863 (16)	0.080 (11)*
O1	0.2756 (2)	0.97875 (15)	1.15499 (10)	0.0522 (5)
O2	0.3166 (2)	0.87012 (16)	0.90634 (11)	0.0608 (6)
C1	0.4721 (3)	0.7357 (2)	1.09042 (16)	0.0566 (8)
H1	0.4859	0.7618	1.0453	0.068*
C2	0.5274 (4)	0.6296 (2)	1.11447 (19)	0.0664 (9)
H2	0.5786	0.5845	1.0854	0.080*
C3	0.5076 (4)	0.5901 (3)	1.18068 (19)	0.0642 (9)
H3	0.5452	0.5185	1.1963	0.077*
C4	0.4320 (4)	0.6564 (3)	1.22422 (17)	0.0617 (8)
H4	0.4183	0.6300	1.2693	0.074*

C5	0.3768 (3)	0.7627 (2)	1.19999 (15)	0.0550 (8)
H5	0.3258	0.8076	1.2293	0.066*
C6	0.3958 (3)	0.8035 (2)	1.13373 (14)	0.0411 (6)
C7	0.3283 (3)	0.9185 (2)	1.11169 (15)	0.0422 (7)
C8	0.2518 (3)	1.0535 (2)	1.01112 (14)	0.0391 (6)
C9	0.2980 (3)	1.1534 (2)	1.04811 (15)	0.0457 (7)
H9	0.3801	1.1528	1.0908	0.055*
C10	0.2238 (3)	1.2540 (2)	1.02250 (15)	0.0481 (7)
C11	0.1031 (3)	1.2557 (2)	0.95916 (16)	0.0487 (7)
C12	0.0627 (3)	1.1572 (2)	0.92025 (15)	0.0461 (7)
H12	−0.0140	1.1594	0.8759	0.055*
C13	0.1339 (3)	1.0549 (2)	0.94576 (14)	0.0400 (6)
C14	0.1654 (3)	0.8714 (2)	0.88694 (14)	0.0433 (7)
C15	0.0737 (3)	0.7775 (2)	0.84321 (14)	0.0432 (7)
C16	−0.0825 (3)	0.7881 (2)	0.79916 (15)	0.0555 (8)
H16	−0.1371	0.8570	0.7957	0.067*
C17	−0.1572 (4)	0.6964 (3)	0.76037 (17)	0.0688 (9)
H17	−0.2616	0.7043	0.7302	0.083*
C18	−0.0799 (4)	0.5938 (3)	0.76558 (18)	0.0667 (9)
H18	−0.1325	0.5320	0.7400	0.080*
C19	0.0747 (4)	0.5828 (3)	0.80849 (19)	0.0678 (9)
H19	0.1280	0.5134	0.8118	0.081*
C20	0.1520 (4)	0.6736 (2)	0.84674 (16)	0.0588 (8)
H20	0.2580	0.6654	0.8753	0.071*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0886 (6)	0.0492 (5)	0.0825 (7)	−0.0102 (4)	0.0100 (5)	−0.0145 (4)
Cl2	0.0950 (7)	0.0447 (5)	0.1010 (8)	0.0163 (4)	−0.0021 (5)	0.0086 (4)
N1	0.0476 (13)	0.0463 (14)	0.0398 (15)	0.0096 (11)	0.0062 (11)	−0.0015 (12)
N2	0.0345 (13)	0.0432 (14)	0.0456 (14)	0.0054 (11)	0.0061 (11)	−0.0046 (10)
O1	0.0583 (12)	0.0532 (12)	0.0451 (12)	0.0122 (10)	0.0113 (9)	−0.0043 (9)
O2	0.0371 (11)	0.0836 (15)	0.0612 (14)	0.0104 (10)	0.0098 (9)	−0.0184 (11)
C1	0.0627 (19)	0.0547 (19)	0.055 (2)	0.0142 (15)	0.0176 (15)	0.0111 (15)
C2	0.075 (2)	0.0536 (19)	0.072 (2)	0.0180 (16)	0.0178 (18)	−0.0005 (17)
C3	0.065 (2)	0.0484 (19)	0.075 (3)	0.0049 (16)	0.0065 (18)	0.0147 (17)
C4	0.064 (2)	0.065 (2)	0.053 (2)	0.0011 (17)	0.0072 (16)	0.0160 (16)
C5	0.0531 (18)	0.064 (2)	0.0459 (19)	0.0053 (15)	0.0075 (14)	0.0056 (15)
C6	0.0344 (14)	0.0453 (16)	0.0415 (17)	0.0027 (12)	0.0040 (12)	−0.0013 (13)
C7	0.0342 (14)	0.0461 (16)	0.0429 (19)	0.0006 (12)	0.0011 (12)	−0.0009 (13)
C8	0.0357 (14)	0.0394 (16)	0.0436 (16)	0.0043 (12)	0.0116 (12)	0.0015 (12)
C9	0.0382 (15)	0.0507 (18)	0.0468 (17)	−0.0040 (13)	0.0064 (12)	−0.0026 (13)
C10	0.0486 (16)	0.0390 (16)	0.058 (2)	−0.0072 (13)	0.0152 (14)	−0.0034 (13)
C11	0.0479 (16)	0.0378 (16)	0.061 (2)	0.0049 (13)	0.0126 (14)	0.0054 (14)
C12	0.0410 (15)	0.0490 (18)	0.0465 (18)	0.0026 (13)	0.0058 (12)	0.0087 (13)
C13	0.0343 (14)	0.0406 (16)	0.0463 (17)	−0.0003 (12)	0.0115 (12)	0.0020 (13)
C14	0.0414 (17)	0.0494 (17)	0.0402 (17)	0.0047 (14)	0.0113 (13)	0.0040 (13)

C15	0.0462 (15)	0.0437 (16)	0.0420 (17)	0.0087 (13)	0.0145 (13)	0.0000 (13)
C16	0.0533 (17)	0.0503 (18)	0.059 (2)	0.0106 (14)	0.0044 (15)	−0.0095 (15)
C17	0.0600 (19)	0.074 (2)	0.068 (2)	0.0023 (18)	0.0029 (16)	−0.0243 (18)
C18	0.080 (2)	0.054 (2)	0.072 (2)	−0.0077 (18)	0.0290 (19)	−0.0220 (17)
C19	0.086 (2)	0.0473 (19)	0.076 (2)	0.0143 (18)	0.0301 (19)	−0.0018 (17)
C20	0.0610 (19)	0.0539 (19)	0.062 (2)	0.0148 (16)	0.0133 (15)	0.0027 (16)

Geometric parameters (Å, °)

Cl1—C10	1.731 (3)	C6—C7	1.498 (3)
Cl2—C11	1.722 (3)	C8—C9	1.384 (3)
N1—C7	1.351 (3)	C8—C13	1.391 (3)
N1—C8	1.418 (3)	C9—C10	1.379 (3)
N1—H1N	0.87 (3)	C9—H9	0.9300
N2—C14	1.355 (3)	C10—C11	1.376 (4)
N2—C13	1.419 (3)	C11—C12	1.379 (3)
N2—H2N	0.85 (3)	C12—C13	1.388 (3)
O1—C7	1.231 (3)	C12—H12	0.9300
O2—C14	1.228 (3)	C14—C15	1.489 (3)
C1—C2	1.381 (4)	C15—C16	1.382 (3)
C1—C6	1.389 (4)	C15—C20	1.388 (3)
C1—H1	0.9300	C16—C17	1.377 (4)
C2—C3	1.369 (4)	C16—H16	0.9300
C2—H2	0.9300	C17—C18	1.369 (4)
C3—C4	1.379 (4)	C17—H17	0.9300
C3—H3	0.9300	C18—C19	1.364 (4)
C4—C5	1.383 (4)	C18—H18	0.9300
C4—H4	0.9300	C19—C20	1.372 (4)
C5—C6	1.373 (3)	C19—H19	0.9300
C5—H5	0.9300	C20—H20	0.9300
C7—N1—C8	124.2 (2)	C11—C10—C9	119.9 (2)
C7—N1—H1N	123.0 (17)	C11—C10—Cl1	121.1 (2)
C8—N1—H1N	112.3 (17)	C9—C10—Cl1	118.9 (2)
C14—N2—C13	126.5 (2)	C10—C11—C12	119.4 (2)
C14—N2—H2N	121 (2)	C10—C11—Cl2	121.3 (2)
C13—N2—H2N	112 (2)	C12—C11—Cl2	119.3 (2)
C2—C1—C6	119.9 (3)	C11—C12—C13	121.5 (2)
C2—C1—H1	120.1	C11—C12—H12	119.3
C6—C1—H1	120.1	C13—C12—H12	119.3
C3—C2—C1	120.7 (3)	C12—C13—C8	118.6 (2)
C3—C2—H2	119.7	C12—C13—N2	117.7 (2)
C1—C2—H2	119.7	C8—C13—N2	123.5 (2)
C2—C3—C4	120.1 (3)	O2—C14—N2	121.9 (2)
C2—C3—H3	120.0	O2—C14—C15	121.3 (2)
C4—C3—H3	120.0	N2—C14—C15	116.7 (2)
C3—C4—C5	119.1 (3)	C16—C15—C20	118.5 (3)
C3—C4—H4	120.5	C16—C15—C14	124.1 (2)
C5—C4—H4	120.5	C20—C15—C14	117.4 (2)
C6—C5—C4	121.5 (3)	C17—C16—C15	120.0 (3)

C6—C5—H5	119.3	C17—C16—H16	120.0
C4—C5—H5	119.3	C15—C16—H16	120.0
C5—C6—C1	118.8 (3)	C18—C17—C16	120.9 (3)
C5—C6—C7	117.4 (2)	C18—C17—H17	119.5
C1—C6—C7	123.8 (3)	C16—C17—H17	119.5
O1—C7—N1	121.9 (2)	C19—C18—C17	119.5 (3)
O1—C7—C6	120.8 (3)	C19—C18—H18	120.2
N1—C7—C6	117.2 (2)	C17—C18—H18	120.2
C9—C8—C13	119.7 (2)	C18—C19—C20	120.4 (3)
C9—C8—N1	119.5 (2)	C18—C19—H19	119.8
C13—C8—N1	120.8 (2)	C20—C19—H19	119.8
C10—C9—C8	120.8 (2)	C19—C20—C15	120.7 (3)
C10—C9—H9	119.6	C19—C20—H20	119.6
C8—C9—H9	119.6	C15—C20—H20	119.6
C6—C1—C2—C3	0.1 (5)	C10—C11—C12—C13	3.9 (4)
C1—C2—C3—C4	−0.1 (5)	Cl2—C11—C12—C13	−176.6 (2)
C2—C3—C4—C5	0.0 (5)	C11—C12—C13—C8	−1.8 (4)
C3—C4—C5—C6	0.0 (4)	C11—C12—C13—N2	174.0 (2)
C4—C5—C6—C1	0.0 (4)	C9—C8—C13—C12	−1.5 (4)
C4—C5—C6—C7	178.6 (2)	N1—C8—C13—C12	176.2 (2)
C2—C1—C6—C5	−0.1 (4)	C9—C8—C13—N2	−177.0 (2)
C2—C1—C6—C7	−178.6 (2)	N1—C8—C13—N2	0.7 (4)
C8—N1—C7—O1	−0.7 (4)	C14—N2—C13—C12	134.9 (3)
C8—N1—C7—C6	176.2 (2)	C14—N2—C13—C8	−49.5 (4)
C5—C6—C7—O1	8.2 (4)	C13—N2—C14—O2	3.5 (4)
C1—C6—C7—O1	−173.3 (3)	C13—N2—C14—C15	−178.4 (2)
C5—C6—C7—N1	−168.7 (2)	O2—C14—C15—C16	−157.0 (3)
C1—C6—C7—N1	9.8 (4)	N2—C14—C15—C16	24.9 (4)
C7—N1—C8—C9	49.1 (4)	O2—C14—C15—C20	22.3 (4)
C7—N1—C8—C13	−128.6 (3)	N2—C14—C15—C20	−155.8 (2)
C13—C8—C9—C10	2.6 (4)	C20—C15—C16—C17	0.4 (4)
N1—C8—C9—C10	−175.1 (2)	C14—C15—C16—C17	179.7 (3)
C8—C9—C10—C11	−0.5 (4)	C15—C16—C17—C18	1.0 (5)
C8—C9—C10—Cl1	−178.9 (2)	C16—C17—C18—C19	−1.5 (5)
C9—C10—C11—C12	−2.8 (4)	C17—C18—C19—C20	0.6 (5)
Cl1—C10—C11—C12	175.6 (2)	C18—C19—C20—C15	0.8 (5)
C9—C10—C11—Cl2	177.8 (2)	C16—C15—C20—C19	−1.3 (4)
Cl1—C10—C11—Cl2	−3.8 (4)	C14—C15—C20—C19	179.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2N···O1^{i}	0.85 (3)	2.15 (3)	2.976 (3)	165 (3)
C5—H5···O1	0.93	2.44	2.769 (3)	101
N1—H1N···O2	0.87 (3)	1.93 (3)	2.702 (3)	147 (2)

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

Fig. 1

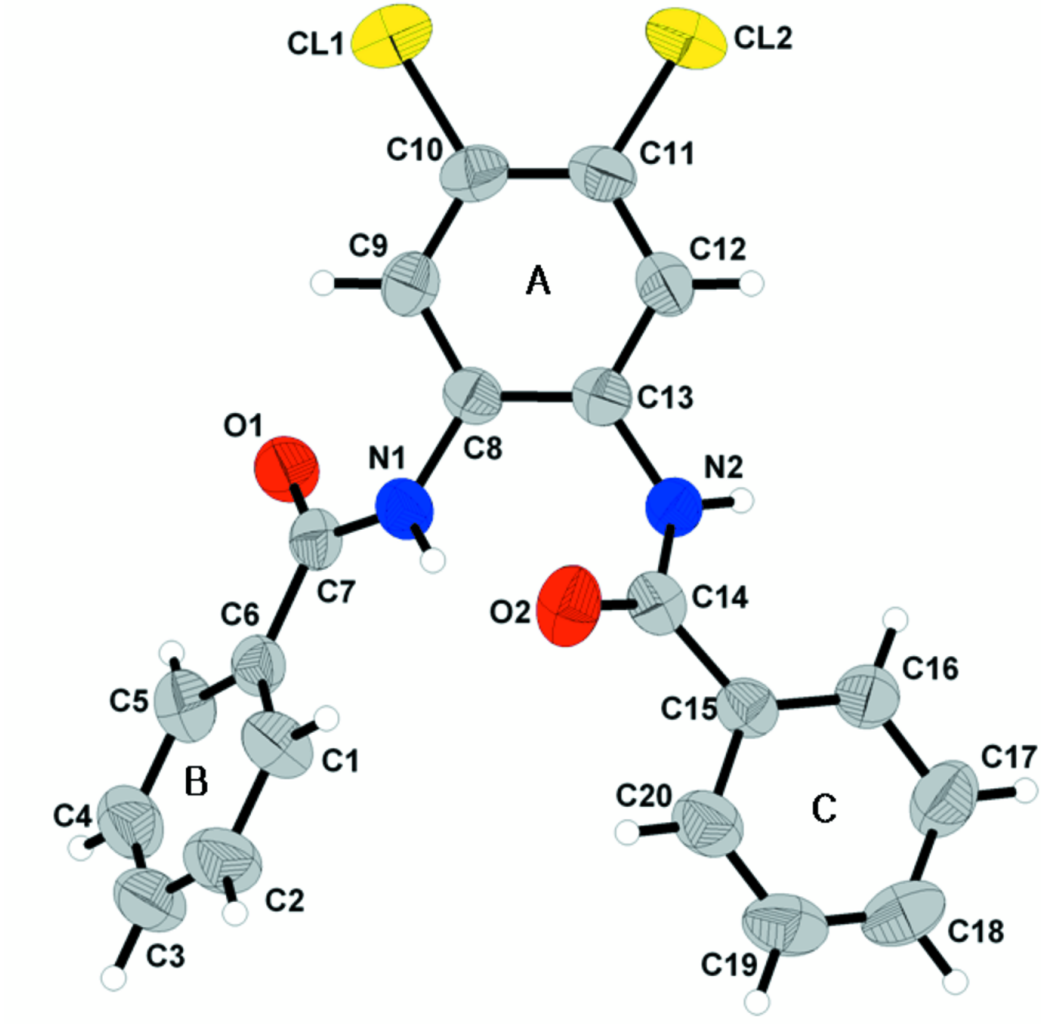
CL1
CL2
C10
C11
C9
C12
A
C13
O1
N1
C8
N2
C7
O2
C14
C6
C16
C5
C15
C1
C17
B
C20
C
C4
C2
C18
C3
C19

Fig. 2