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2-(4,5,6,7-Tetrachloro-1,3-dioxoisoindolin-2-yl)benzoic acid *N*,*N*-dimethylformamide solvate

Jian Li

Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China
Correspondence e-mail: ljwfu@163.com

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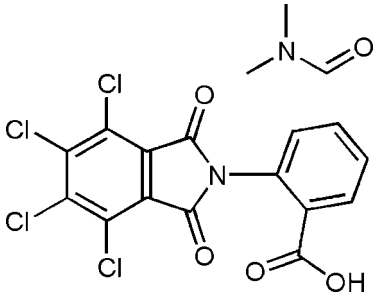
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.054; wR factor = 0.121; data-to-parameter ratio = 13.3.

In the crystal structure of the title compound, $C_{15}H_5Cl_4NO_4\cdot C_3H_7NO$, O—H···O hydrogen bonds help to establish the crystal packing. The dihedral angle between the tetrachlorophthalimide group and the benzene ring is 74.2 (2)°.

Related literature

For related literature, see: Liang *et al.* (2006, 2007); Lima *et al.* (2002).



Experimental

Crystal data

$C_{15}H_5Cl_4NO_4\cdot C_3H_7NO$
M_r = 478.10
Monoclinic, $P2_1/c$
a = 16.593 (4) Å
b = 13.816 (3) Å
c = 8.815 (2) Å
β = 98.224 (3)°
V = 2000.1 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 298 (2) K
0.44 × 0.10 × 0.05 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.770, T_{max} = 0.969
8292 measured reflections
3528 independent reflections
2587 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.121
S = 1.09
3528 reflections
265 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 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
O4—H4···O5^{i}	0.82	1.76	2.574 (4)	169

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

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, 1997); 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: HB2454).

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supplementary materials

Acta Cryst. (2007). E**63**, o3332 [**doi:10.1107/S1600536807030644**]

2-(4,5,6,7-Tetrachloro-1,3-dioxoisoindolin-2-yl)benzoic acid *N*,*N*-dimethylformamide solvate

J. Li

Comment

Phthalimides and N-substituted phthalimides are an important class of compounds because of their interesting biological activities (Lima *et al.*, 2002). In this paper, the structure of the title compound, (I), is reported. The asymmetric unit of (I) contains one 2-(4,5,6,7-tetrachloro-1,3-dioxoisoindolin-2-yl)benzoic acid molecule and one DMF molecule (Fig. 1). The bond lengths and angles agree with those in those similar compounds 4-Phthalimidobenzoic acid *N*,*N*-dimethylformamide solvate (Liang *et al.*, 2006) and 4-(5-Bromo-1,3-dioxoisoindolin-2-yl)benzoic acid *N*,*N*-dimethylformamide solvate (Liang *et al.*, 2007). The tetrachlorophthalimide group is essentially planar, with a mean deviation of 0.424 (3) Å. The dihedral angle between the tetrachlorophthalimide group and the benzene C9—C14 ring is 74.2 (2) °. The DMF molecule is planar, within 0.009 (2) Å, for all non-H atoms. The crystal structure is stabilized by an O—H···O hydrogen bond which connects the benzoic acid and DMF molecules (Fig. 2 and Table 1).

Experimental

A mixture of 4,5,6,7-tetrachloroisobenzofuran-1,3-dione (0.01 mol) and 2-aminobenzoic acid (0.01 mol) in acetic acid (10 ml) was refluxed for 1 h. After cooling, filtration and drying, 2-(4,5,6,7-tetrachloro-1,3-dioxoisoindolin-2-yl)benzoic acid was obtained. 10 mg of this compound was dissolved in DMF (7 ml), and the solution was kept at room temperature for 5 d. Natural evaporation gave colourless bars of (I).

Refinement

The H atoms were initially located from difference maps, then relocated in idealized locations (C—H = 0.93–0.96 Å, O—H = 0.82 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(O, methyl-C).

Figures

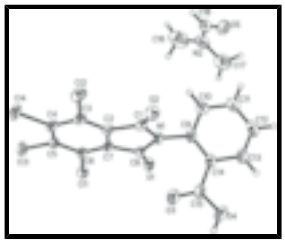

Fig. 1. The molecular structure of (I), drawn with 30% probability ellipsoids (arbitrary spheres for the H atoms).

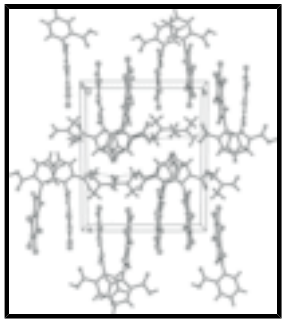

Fig. 2. The crystal packing of (I), viewed along the *c* axis. Hydrogen bonds are indicated by dashed lines.

2-(4,5,6,7-Tetrachloro-1,3-dioxoisoindolin-2-yl)benzoic acid *N*,*N*-dimethylformamide solvate

Crystal data

$C_{15}H_5Cl_4NO_4 \cdot C_3H_7NO$	$F_{000} = 968$
$M_r = 478.10$	$D_x = 1.588$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1625 reflections
$a = 16.593$ (4) Å	$\theta = 2.8$–21.0º
$b = 13.816$ (3) Å	$\mu = 0.63$ mm^{-1}
$c = 8.815$ (2) Å	$T = 298$ (2) K
$\beta = 98.224$ (3)º	Bar, colourless
$V = 2000.1$ (8) Å^3	0.44 × 0.10 × 0.05 mm
$Z = 4$	

Data collection

Bruker SMART CCD diffractometer	3528 independent reflections
Radiation source: fine-focus sealed tube	2587 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.040$
$T = 298$(2) K	$\theta_{max} = 25.0$º
ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -19 \rightarrow 19$
$T_{min} = 0.770$, $T_{max} = 0.969$	$k = -16 \rightarrow 14$
8292 measured reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.121$	$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.09	$(\Delta/\sigma)_{max}$ = 0.001
3528 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
265 parameters	$\Delta\rho_{min}$ = −0.23 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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.78652 (19)	0.8663 (2)	0.5252 (4)	0.0391 (8)
C2	0.87721 (18)	0.8736 (2)	0.5443 (4)	0.0361 (7)
C3	0.9324 (2)	0.8832 (2)	0.6743 (4)	0.0407 (8)
C4	1.0152 (2)	0.8842 (2)	0.6598 (4)	0.0420 (8)
C5	1.03952 (18)	0.8758 (2)	0.5153 (4)	0.0402 (8)
C6	0.98224 (18)	0.8674 (2)	0.3831 (4)	0.0362 (7)
C7	0.90112 (17)	0.8657 (2)	0.4001 (3)	0.0335 (7)
C8	0.82696 (18)	0.8506 (2)	0.2852 (4)	0.0353 (7)
C9	0.67996 (18)	0.8270 (2)	0.3073 (4)	0.0419 (8)
C10	0.6508 (2)	0.7372 (3)	0.3368 (4)	0.0573 (10)
H10	0.6842	0.6933	0.3960	0.069*
C11	0.5722 (2)	0.7120 (3)	0.2789 (5)	0.0661 (11)
H11	0.5524	0.6512	0.2996	0.079*
C12	0.5232 (2)	0.7764 (3)	0.1909 (5)	0.0658 (12)
H12	0.4704	0.7588	0.1500	0.079*
C13	0.5518 (2)	0.8662 (3)	0.1634 (4)	0.0585 (10)
H13	0.5179	0.9094	0.1038	0.070*
C14	0.63042 (19)	0.8948 (2)	0.2221 (4)	0.0452 (9)
C15	0.6573 (2)	0.9951 (3)	0.1991 (5)	0.0571 (10)
C16	0.7469 (4)	0.4024 (4)	0.3307 (6)	0.128 (2)
H16A	0.7796	0.3524	0.3842	0.192*
H16B	0.7180	0.4364	0.4012	0.192*
H16C	0.7814	0.4468	0.2862	0.192*
C17	0.6316 (3)	0.4208 (4)	0.1177 (8)	0.124 (2)
H17A	0.6535	0.4397	0.0272	0.186*
H17B	0.6212	0.4774	0.1751	0.186*
H17C	0.5816	0.3861	0.0891	0.186*

C18	0.6885 (3)	0.2661 (4)	0.1868 (6)	0.0765 (13)
H18	0.7250	0.2281	0.2512	0.092*
Cl1	1.01316 (5)	0.86077 (6)	0.20580 (10)	0.0486 (3)
Cl2	0.90173 (6)	0.88868 (7)	0.85233 (10)	0.0573 (3)
Cl3	1.14152 (5)	0.87399 (7)	0.50024 (12)	0.0597 (3)
Cl4	1.08683 (6)	0.89372 (8)	0.81974 (11)	0.0669 (3)
N1	0.76245 (14)	0.84798 (18)	0.3700 (3)	0.0387 (6)
N2	0.6890 (2)	0.3596 (3)	0.2105 (5)	0.0793 (11)
O1	0.82200 (13)	0.83982 (17)	0.1491 (3)	0.0497 (6)
O2	0.74198 (14)	0.87608 (17)	0.6190 (3)	0.0553 (7)
O3	0.71942 (17)	1.0292 (2)	0.2590 (4)	0.0976 (11)
O4	0.60601 (17)	1.0458 (2)	0.1063 (4)	0.1018 (11)
H4	0.6238	1.1008	0.0999	0.153*
O5	0.64297 (19)	0.2258 (2)	0.0852 (4)	0.0922 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0441 (19)	0.0397 (19)	0.033 (2)	0.0051 (15)	0.0016 (16)	0.0035 (15)
C2	0.0414 (18)	0.0324 (17)	0.0332 (19)	0.0051 (14)	0.0009 (15)	0.0028 (14)
C3	0.053 (2)	0.0376 (19)	0.0289 (19)	0.0027 (15)	−0.0018 (16)	0.0025 (14)
C4	0.050 (2)	0.0359 (19)	0.035 (2)	0.0018 (14)	−0.0121 (16)	0.0009 (15)
C5	0.0363 (18)	0.0358 (18)	0.045 (2)	0.0008 (14)	−0.0051 (16)	0.0015 (15)
C6	0.0375 (18)	0.0369 (18)	0.0328 (19)	0.0017 (14)	0.0000 (14)	−0.0002 (15)
C7	0.0344 (17)	0.0361 (17)	0.0279 (18)	0.0009 (13)	−0.0025 (13)	0.0015 (14)
C8	0.0353 (18)	0.0395 (19)	0.029 (2)	−0.0020 (14)	−0.0014 (14)	0.0026 (15)
C9	0.0340 (18)	0.057 (2)	0.034 (2)	−0.0011 (16)	0.0033 (15)	−0.0030 (17)
C10	0.051 (2)	0.064 (3)	0.057 (3)	−0.0038 (19)	0.008 (2)	0.008 (2)
C11	0.059 (3)	0.065 (3)	0.076 (3)	−0.017 (2)	0.016 (2)	0.002 (2)
C12	0.040 (2)	0.083 (3)	0.074 (3)	−0.018 (2)	0.008 (2)	−0.009 (2)
C13	0.037 (2)	0.080 (3)	0.056 (3)	−0.0026 (19)	−0.0020 (18)	0.002 (2)
C14	0.0341 (19)	0.058 (2)	0.042 (2)	−0.0014 (16)	0.0011 (16)	−0.0035 (18)
C15	0.037 (2)	0.067 (3)	0.063 (3)	0.0055 (19)	−0.0071 (19)	0.002 (2)
C16	0.173 (6)	0.126 (5)	0.086 (4)	−0.074 (4)	0.017 (4)	−0.020 (4)
C17	0.114 (5)	0.071 (4)	0.188 (7)	−0.007 (3)	0.022 (5)	0.025 (4)
C18	0.061 (3)	0.085 (4)	0.080 (4)	−0.012 (3)	0.001 (2)	0.008 (3)
Cl1	0.0435 (5)	0.0632 (6)	0.0394 (5)	−0.0020 (4)	0.0074 (4)	−0.0041 (4)
Cl2	0.0743 (7)	0.0680 (6)	0.0273 (5)	0.0027 (5)	−0.0004 (4)	−0.0017 (4)
Cl3	0.0336 (5)	0.0709 (6)	0.0704 (7)	0.0007 (4)	−0.0074 (4)	−0.0015 (5)
Cl4	0.0632 (6)	0.0823 (7)	0.0454 (6)	−0.0003 (5)	−0.0254 (5)	−0.0032 (5)
N1	0.0289 (14)	0.0557 (17)	0.0305 (16)	0.0001 (12)	0.0007 (12)	0.0019 (13)
N2	0.084 (3)	0.072 (3)	0.084 (3)	−0.023 (2)	0.020 (2)	0.002 (2)
O1	0.0419 (14)	0.0784 (17)	0.0278 (14)	−0.0075 (11)	0.0015 (10)	−0.0054 (12)
O2	0.0528 (15)	0.0754 (18)	0.0395 (15)	0.0042 (12)	0.0125 (12)	−0.0052 (13)
O3	0.066 (2)	0.072 (2)	0.136 (3)	−0.0150 (16)	−0.0480 (19)	0.0227 (19)
O4	0.070 (2)	0.074 (2)	0.141 (3)	−0.0064 (16)	−0.0514 (19)	0.035 (2)
O5	0.087 (2)	0.073 (2)	0.107 (3)	0.0002 (17)	−0.020 (2)	0.0049 (19)

Geometric parameters (Å, °)

C1—O2	1.193 (3)	C11—C12	1.369 (5)
C1—N1	1.392 (4)	C11—H11	0.9300
C1—C2	1.494 (4)	C12—C13	1.363 (5)
C2—C3	1.367 (4)	C12—H12	0.9300
C2—C7	1.389 (4)	C13—C14	1.390 (5)
C3—C4	1.398 (4)	C13—H13	0.9300
C3—Cl2	1.719 (3)	C14—C15	1.478 (5)
C4—C5	1.395 (5)	C15—O3	1.187 (4)
C4—Cl4	1.714 (3)	C15—O4	1.298 (4)
C5—C6	1.399 (4)	C16—N2	1.451 (6)
C5—Cl3	1.717 (3)	C16—H16A	0.9600
C6—C7	1.376 (4)	C16—H16B	0.9600
C6—Cl1	1.716 (3)	C16—H16C	0.9600
C7—C8	1.493 (4)	C17—N2	1.439 (6)
C8—O1	1.200 (3)	C17—H17A	0.9600
C8—N1	1.391 (4)	C17—H17B	0.9600
C9—C10	1.370 (4)	C17—H17C	0.9600
C9—C14	1.393 (4)	C18—O5	1.220 (5)
C9—N1	1.431 (4)	C18—N2	1.308 (5)
C10—C11	1.376 (5)	C18—H18	0.9300
C10—H10	0.9300	O4—H4	0.8200
?···?	?		
O2—C1—N1	125.6 (3)	C13—C12—H12	120.1
O2—C1—C2	128.9 (3)	C11—C12—H12	120.1
N1—C1—C2	105.4 (3)	C12—C13—C14	121.7 (4)
C3—C2—C7	122.0 (3)	C12—C13—H13	119.1
C3—C2—C1	130.2 (3)	C14—C13—H13	119.1
C7—C2—C1	107.8 (3)	C13—C14—C9	117.3 (3)
C2—C3—C4	118.3 (3)	C13—C14—C15	120.1 (3)
C2—C3—Cl2	121.2 (3)	C9—C14—C15	122.5 (3)
C4—C3—Cl2	120.4 (3)	O3—C15—O4	121.1 (4)
C5—C4—C3	119.9 (3)	O3—C15—C14	124.8 (4)
C5—C4—Cl4	120.0 (3)	O4—C15—C14	114.2 (3)
C3—C4—Cl4	120.0 (3)	N2—C16—H16A	109.5
C4—C5—C6	121.1 (3)	N2—C16—H16B	109.5
C4—C5—Cl3	119.3 (3)	H16A—C16—H16B	109.5
C6—C5—Cl3	119.6 (3)	N2—C16—H16C	109.5
C7—C6—C5	118.0 (3)	H16A—C16—H16C	109.5
C7—C6—Cl1	121.5 (2)	H16B—C16—H16C	109.5
C5—C6—Cl1	120.5 (2)	N2—C17—H17A	109.5
C6—C7—C2	120.7 (3)	N2—C17—H17B	109.5
C6—C7—C8	130.8 (3)	H17A—C17—H17B	109.5
C2—C7—C8	108.5 (3)	N2—C17—H17C	109.5
O1—C8—N1	125.9 (3)	H17A—C17—H17C	109.5
O1—C8—C7	128.9 (3)	H17B—C17—H17C	109.5
N1—C8—C7	105.2 (3)	O5—C18—N2	123.8 (5)

C10—C9—C14	120.9 (3)	O5—C18—H18	118.1
C10—C9—N1	117.0 (3)	N2—C18—H18	118.1
C14—C9—N1	122.0 (3)	C8—N1—C1	112.9 (3)
C9—C10—C11	120.1 (4)	C8—N1—C9	124.4 (3)
C9—C10—H10	120.0	C1—N1—C9	122.7 (3)
C11—C10—H10	120.0	C18—N2—C17	120.1 (4)
C12—C11—C10	120.0 (4)	C18—N2—C16	120.5 (5)
C12—C11—H11	120.0	C17—N2—C16	119.4 (5)
C10—C11—H11	120.0	C15—O4—H4	109.5
C13—C12—C11	119.9 (4)		
O2—C1—C2—C3	7.5 (5)	C2—C7—C8—N1	−1.5 (3)
N1—C1—C2—C3	−174.2 (3)	C14—C9—C10—C11	1.6 (5)
O2—C1—C2—C7	−174.5 (3)	N1—C9—C10—C11	−179.5 (3)
N1—C1—C2—C7	3.8 (3)	C9—C10—C11—C12	0.4 (6)
C7—C2—C3—C4	−0.5 (4)	C10—C11—C12—C13	−1.3 (6)
C1—C2—C3—C4	177.2 (3)	C11—C12—C13—C14	0.2 (6)
C7—C2—C3—Cl2	−177.7 (2)	C12—C13—C14—C9	1.7 (5)
C1—C2—C3—Cl2	0.1 (5)	C12—C13—C14—C15	−175.6 (3)
C2—C3—C4—C5	0.2 (4)	C10—C9—C14—C13	−2.6 (5)
Cl2—C3—C4—C5	177.4 (2)	N1—C9—C14—C13	178.5 (3)
C2—C3—C4—Cl4	−178.7 (2)	C10—C9—C14—C15	174.6 (3)
Cl2—C3—C4—Cl4	−1.5 (4)	N1—C9—C14—C15	−4.3 (5)
C3—C4—C5—C6	0.7 (5)	C13—C14—C15—O3	171.1 (4)
Cl4—C4—C5—C6	179.6 (2)	C9—C14—C15—O3	−6.0 (6)
C3—C4—C5—Cl3	−178.3 (2)	C13—C14—C15—O4	−8.4 (5)
Cl4—C4—C5—Cl3	0.6 (4)	C9—C14—C15—O4	174.5 (4)
C4—C5—C6—C7	−1.3 (4)	O1—C8—N1—C1	−177.8 (3)
Cl3—C5—C6—C7	177.7 (2)	C7—C8—N1—C1	4.1 (3)
C4—C5—C6—Cl1	178.0 (2)	O1—C8—N1—C9	3.3 (5)
Cl3—C5—C6—Cl1	−3.0 (4)	C7—C8—N1—C9	−174.8 (3)
C5—C6—C7—C2	1.0 (4)	O2—C1—N1—C8	173.4 (3)
Cl1—C6—C7—C2	−178.3 (2)	C2—C1—N1—C8	−4.9 (3)
C5—C6—C7—C8	−175.1 (3)	O2—C1—N1—C9	−7.7 (5)
Cl1—C6—C7—C8	5.6 (5)	C2—C1—N1—C9	173.9 (3)
C3—C2—C7—C6	−0.1 (4)	C10—C9—N1—C8	104.9 (3)
C1—C2—C7—C6	−178.3 (3)	C14—C9—N1—C8	−76.2 (4)
C3—C2—C7—C8	176.8 (3)	C10—C9—N1—C1	−73.9 (4)
C1—C2—C7—C8	−1.4 (3)	C14—C9—N1—C1	105.0 (4)
C6—C7—C8—O1	−3.0 (5)	O5—C18—N2—C17	2.4 (7)
C2—C7—C8—O1	−179.5 (3)	O5—C18—N2—C16	−178.0 (4)
C6—C7—C8—N1	175.0 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O5^{i}	0.82	1.76	2.574 (4)	169

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

Fig. 1

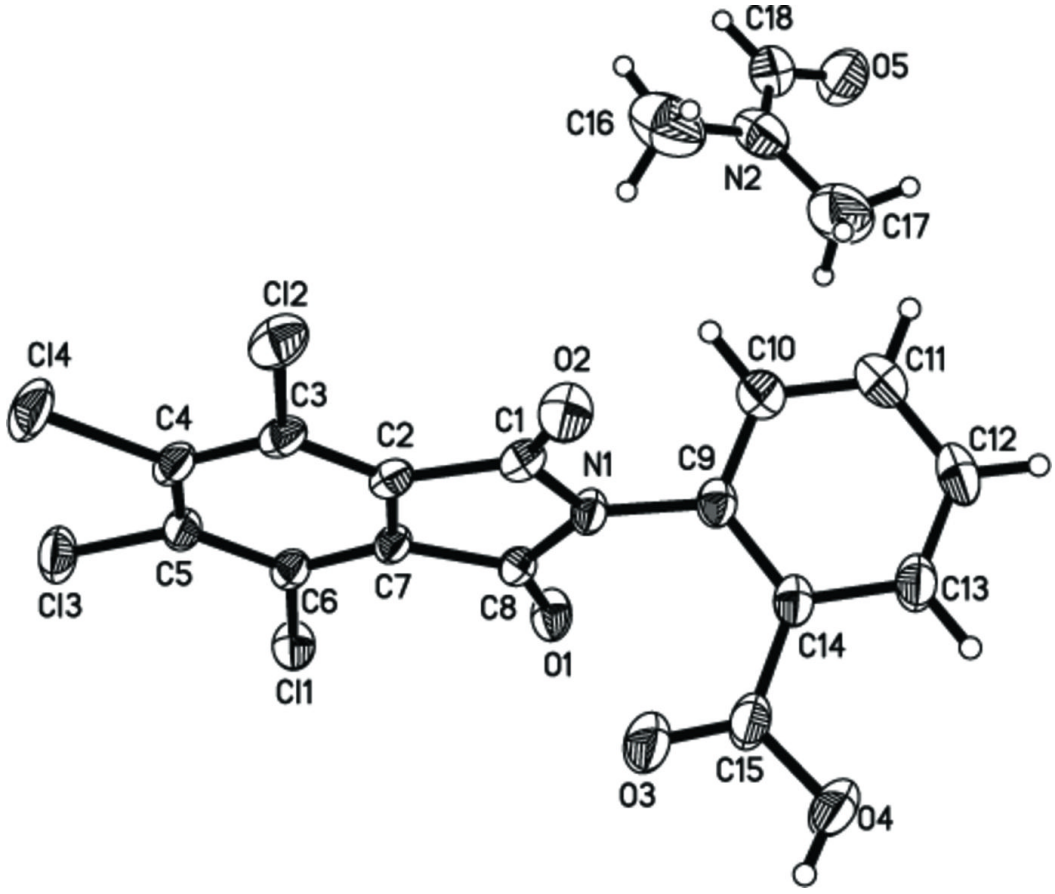
C18
O5
C16
N2
C17
Cl2
Cl4
C3
O2
C10
C11
C4
C2
C1
C12
N1
C9
Cl3
C5
C6
C7
C8
C13
O1
C14
Cl1
O3
C15
O4

Fig. 2