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4,5,6,7-Tetrachloro-2-phenylisoindoline-1,3-dione

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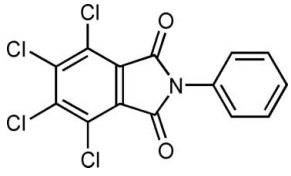
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.117; data-to-parameter ratio = 13.1.

In the title compound, $C_{14}H_5Cl_4NO_2$, the tetrachlorophthalimide group is planar to within 0.037 (3) Å and forms a dihedral angle of 61.6 (2)° with the phenyl substituent.

Related literature

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



Experimental

Crystal data

$C_{14}H_5Cl_4NO_2$
M_r = 360.99
Orthorhombic, *Pbca*
a = 16.854 (5) Å
b = 6.780 (2) Å
c = 24.749 (8) Å
V = 2828.0 (15) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.84 mm^{-1}
T = 298 (2) K
0.49 × 0.42 × 0.01 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.684, T_{max} = 0.992
11041 measured reflections
2484 independent reflections
2131 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.117
S = 1.09
2484 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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: BI2206).

References

Bruker (1997). *SADABS* (Version 2.01), *SMART* (Version 5.044), *SAINT* (Version 5.01) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Li, J., Liang, Z.-P. & Wang, H.-Q. (2007). *Acta Cryst.* E**63**, o627–o628.
Liang, Z.-P. & Li, J. (2006). *Acta Cryst.* E**62**, o4436–o4437.
Lima, L. M., Castro, P., Machado, A. L., Frage, C. A. M., Lugnier, C., Gonçalves de Moraes, V. L. & Barreiro, E. J. (2002). *Bioorg. Med. Chem.* **10**, 3067–3073.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

Acta Cryst. (2007). E**63**, o3515 [**doi:10.1107/S1600536807034290**]

4,5,6,7-Tetrachloro-2-phenylisoindoline-1,3-dione

J. Li

Comment

Phthalimides and *N*-substituted phthalimides are an important class of compounds because of their interesting biological activities (Lima *et al.*, 2002). The molecular structure of the title compound (Figure 1) is similar to the related compounds 2-(2-hydroxyphenyl)isoindoline-1,3-dione (Li *et al.*, 2007) and 2-(4-hydroxyphenyl)isoindoline-1,3-dione (Liang & Li, 2006). The tetrachlorophthalimide moiety system is planar to within 0.037 (3) Å. The dihedral angle between the phenyl ring and the tetrachlorophthalimide moiety is 61.6 (2) °.

Experimental

A mixture of 4,5,6,7-tetrachloroisobenzofuran-1,3-dione (0.01 mol) and aniline (0.01 mol) in acetic acid (10 ml) was refluxed for 1 h. After cooling, filtration and drying, the title compound was obtained. Single crystals suitable for X-ray analysis were obtained by slow evaporation from a solution of 10 mg in 15 ml acetone.

Refinement

H atoms were visible in difference Fourier maps but were placed geometrically and refined using a riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

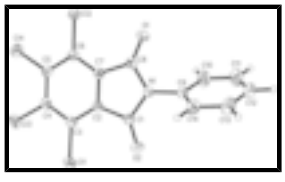

Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at 30% probability for non-H atoms.

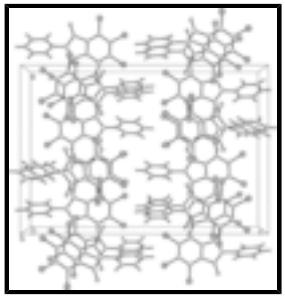

Fig. 2. Packing of the title compound viewed along the *b* axis.

4,5,6,7-Tetrachloro-2-phenylisoindoline-1,3-dione

Crystal data

$C_{14}H_5Cl_4NO_2$	F_{000} = 1440
M_r = 360.99	D_x = 1.696 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 4222 reflections
a = 16.854 (5) Å	θ = 2.4–27.3º
b = 6.780 (2) Å	μ = 0.84 mm^{-1}
c = 24.749 (8) Å	*T* = 298 (2) K
V = 2828.0 (15) Å^3	Plate, colourless
Z = 8	0.49 × 0.42 × 0.01 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2484 independent reflections
Radiation source: fine-focus sealed tube	2131 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	*h* = −19→20
T_{min} = 0.684, T_{max} = 0.992	*k* = −7→8
11041 measured reflections	*l* = −17→29

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.042	H-atom parameters constrained
$wR(F^2)$ = 0.117	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 0.5952P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.09	$(\Delta/\sigma)_{max}$ = 0.001
2484 reflections	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
190 parameters	$\Delta\rho_{min}$ = −0.38 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	0.70198 (16)	−0.0160 (3)	0.79596 (10)	0.0354 (6)
C2	0.67110 (14)	0.0075 (3)	0.73988 (10)	0.0316 (5)
C3	0.71096 (15)	0.0256 (3)	0.69145 (10)	0.0328 (6)
C4	0.66528 (16)	0.0442 (3)	0.64456 (10)	0.0344 (6)
C5	0.58288 (16)	0.0397 (3)	0.64655 (10)	0.0366 (6)
C6	0.54312 (15)	0.0189 (3)	0.69589 (10)	0.0336 (6)
C7	0.58916 (15)	0.0068 (3)	0.74209 (10)	0.0316 (5)
C8	0.56418 (16)	−0.0068 (3)	0.79972 (10)	0.0356 (6)
C9	0.63664 (15)	−0.0407 (4)	0.88692 (10)	0.0405 (6)
C10	0.6026 (2)	0.1018 (6)	0.91814 (13)	0.0715 (10)
H10	0.5814	0.2148	0.9025	0.086*
C11	0.6002 (3)	0.0752 (7)	0.97342 (15)	0.0969 (15)
H11	0.5767	0.1708	0.9951	0.116*
C12	0.6312 (2)	−0.0859 (8)	0.99626 (14)	0.0886 (15)
H12	0.6286	−0.1027	1.0335	0.106*
C13	0.6665 (2)	−0.2253 (7)	0.96492 (13)	0.0807 (11)
H13	0.6891	−0.3358	0.9810	0.097*
C14	0.66904 (18)	−0.2043 (5)	0.90959 (11)	0.0576 (8)
H14	0.6925	−0.3005	0.8881	0.069*
Cl1	0.81288 (4)	0.02580 (9)	0.68847 (3)	0.0411 (2)
Cl2	0.44169 (4)	0.00610 (9)	0.69857 (3)	0.0426 (2)
Cl3	0.71186 (5)	0.07602 (11)	0.58370 (3)	0.0524 (2)
Cl4	0.52839 (5)	0.06222 (12)	0.58853 (3)	0.0583 (3)
N1	0.63480 (12)	−0.0189 (3)	0.82904 (8)	0.0355 (5)
O1	0.49834 (11)	−0.0061 (3)	0.81870 (8)	0.0469 (5)
O2	0.76928 (11)	−0.0317 (3)	0.81109 (8)	0.0506 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0304 (14)	0.0362 (13)	0.0395 (14)	−0.0002 (10)	0.0002 (10)	−0.0060 (10)
C2	0.0314 (13)	0.0274 (11)	0.0360 (13)	0.0001 (9)	0.0016 (10)	−0.0046 (9)
C3	0.0324 (14)	0.0257 (11)	0.0402 (13)	−0.0033 (9)	0.0063 (10)	−0.0039 (9)
C4	0.0430 (15)	0.0268 (11)	0.0334 (13)	−0.0027 (10)	0.0068 (10)	−0.0013 (9)
C5	0.0436 (15)	0.0328 (12)	0.0333 (13)	−0.0025 (10)	−0.0010 (11)	0.0017 (10)
C6	0.0306 (13)	0.0349 (12)	0.0352 (13)	−0.0003 (10)	−0.0012 (10)	0.0016 (10)
C7	0.0323 (13)	0.0288 (11)	0.0337 (13)	0.0002 (10)	0.0022 (10)	−0.0016 (9)

C8	0.0328 (14)	0.0376 (14)	0.0365 (14)	0.0017 (10)	0.0006 (10)	−0.0011 (10)
C9	0.0327 (14)	0.0577 (16)	0.0311 (14)	0.0015 (11)	−0.0026 (10)	−0.0010 (12)
C10	0.080 (2)	0.087 (3)	0.0481 (19)	0.030 (2)	−0.0025 (16)	−0.0151 (17)
C11	0.089 (3)	0.153 (4)	0.049 (2)	0.035 (3)	0.0008 (19)	−0.036 (2)
C12	0.056 (2)	0.178 (5)	0.0313 (17)	−0.003 (2)	−0.0056 (15)	0.001 (2)
C13	0.074 (2)	0.118 (3)	0.050 (2)	0.007 (2)	−0.0165 (18)	0.023 (2)
C14	0.0558 (19)	0.073 (2)	0.0437 (16)	0.0088 (16)	−0.0079 (13)	0.0015 (15)
Cl1	0.0323 (4)	0.0385 (4)	0.0525 (4)	−0.0027 (2)	0.0088 (3)	−0.0040 (3)
Cl2	0.0297 (4)	0.0531 (4)	0.0449 (4)	−0.0008 (3)	−0.0031 (3)	0.0048 (3)
Cl3	0.0569 (5)	0.0617 (5)	0.0385 (4)	−0.0062 (3)	0.0141 (3)	0.0020 (3)
Cl4	0.0550 (5)	0.0834 (6)	0.0366 (4)	−0.0083 (4)	−0.0076 (3)	0.0101 (3)
N1	0.0315 (12)	0.0448 (12)	0.0303 (11)	0.0007 (8)	0.0001 (8)	−0.0016 (9)
O1	0.0303 (11)	0.0689 (12)	0.0416 (10)	0.0014 (8)	0.0054 (8)	0.0026 (9)
O2	0.0302 (11)	0.0744 (13)	0.0472 (11)	0.0012 (9)	−0.0033 (8)	−0.0032 (9)

Geometric parameters (Å, °)

C1—O2	1.199 (3)	C8—O1	1.205 (3)
C1—N1	1.398 (3)	C8—N1	1.396 (3)
C1—C2	1.491 (4)	C9—C14	1.358 (4)
C2—C3	1.379 (3)	C9—C10	1.364 (4)
C2—C7	1.382 (4)	C9—N1	1.440 (3)
C3—C4	1.398 (4)	C10—C11	1.381 (5)
C3—Cl1	1.719 (3)	C10—H10	0.930
C4—C5	1.390 (4)	C11—C12	1.336 (6)
C4—Cl3	1.712 (2)	C11—H11	0.930
C5—C6	1.400 (4)	C12—C13	1.360 (5)
C5—Cl4	1.711 (3)	C12—H12	0.930
C6—C7	1.384 (4)	C13—C14	1.377 (4)
C6—Cl2	1.713 (3)	C13—H13	0.930
C7—C8	1.490 (3)	C14—H14	0.930
O2—C1—N1	125.6 (2)	N1—C8—C7	105.1 (2)
O2—C1—C2	129.1 (2)	C14—C9—C10	120.9 (3)
N1—C1—C2	105.3 (2)	C14—C9—N1	120.2 (2)
C3—C2—C7	121.4 (2)	C10—C9—N1	118.8 (3)
C3—C2—C1	130.4 (2)	C9—C10—C11	118.8 (3)
C7—C2—C1	108.2 (2)	C9—C10—H10	120.6
C2—C3—C4	117.5 (2)	C11—C10—H10	120.6
C2—C3—Cl1	121.6 (2)	C12—C11—C10	121.0 (4)
C4—C3—Cl1	120.96 (19)	C12—C11—H11	119.5
C5—C4—C3	121.2 (2)	C10—C11—H11	119.5
C5—C4—Cl3	119.49 (18)	C11—C12—C13	119.9 (3)
C3—C4—Cl3	119.3 (2)	C11—C12—H12	120.1
C4—C5—C6	120.8 (2)	C13—C12—H12	120.1
C4—C5—Cl4	120.29 (18)	C12—C13—C14	120.6 (4)
C6—C5—Cl4	118.9 (2)	C12—C13—H13	119.7
C7—C6—C5	117.3 (2)	C14—C13—H13	119.7
C7—C6—Cl2	121.64 (19)	C9—C14—C13	118.9 (3)
C5—C6—Cl2	121.1 (2)	C9—C14—H14	120.6

C2—C7—C6	121.8 (2)	C13—C14—H14	120.6
C2—C7—C8	108.7 (2)	C8—N1—C1	112.7 (2)
C6—C7—C8	129.5 (2)	C8—N1—C9	122.8 (2)
O1—C8—N1	125.6 (2)	C1—N1—C9	124.5 (2)
O1—C8—C7	129.3 (2)		
O2—C1—C2—C3	−3.1 (4)	C5—C6—C7—C8	177.0 (2)
N1—C1—C2—C3	177.6 (2)	Cl2—C6—C7—C8	−3.7 (3)
O2—C1—C2—C7	176.2 (2)	C2—C7—C8—O1	177.8 (2)
N1—C1—C2—C7	−3.1 (2)	C6—C7—C8—O1	−1.7 (4)
C7—C2—C3—C4	0.3 (3)	C2—C7—C8—N1	−1.5 (2)
C1—C2—C3—C4	179.5 (2)	C6—C7—C8—N1	178.9 (2)
C7—C2—C3—Cl1	−179.80 (16)	C14—C9—C10—C11	−1.2 (5)
C1—C2—C3—Cl1	−0.6 (3)	N1—C9—C10—C11	176.2 (3)
C2—C3—C4—C5	−1.5 (3)	C9—C10—C11—C12	0.6 (7)
Cl1—C3—C4—C5	178.53 (17)	C10—C11—C12—C13	0.8 (7)
C2—C3—C4—Cl3	177.68 (17)	C11—C12—C13—C14	−1.5 (6)
Cl1—C3—C4—Cl3	−2.3 (3)	C10—C9—C14—C13	0.5 (5)
C3—C4—C5—C6	0.8 (3)	N1—C9—C14—C13	−176.9 (3)
Cl3—C4—C5—C6	−178.38 (18)	C12—C13—C14—C9	0.9 (5)
C3—C4—C5—Cl4	−179.87 (18)	O1—C8—N1—C1	−179.9 (2)
Cl3—C4—C5—Cl4	0.9 (3)	C7—C8—N1—C1	−0.5 (3)
C4—C5—C6—C7	1.1 (3)	O1—C8—N1—C9	2.7 (4)
Cl4—C5—C6—C7	−178.17 (17)	C7—C8—N1—C9	−178.0 (2)
C4—C5—C6—Cl2	−178.12 (16)	O2—C1—N1—C8	−177.1 (2)
Cl4—C5—C6—Cl2	2.6 (3)	C2—C1—N1—C8	2.2 (3)
C3—C2—C7—C6	1.8 (3)	O2—C1—N1—C9	0.3 (4)
C1—C2—C7—C6	−177.6 (2)	C2—C1—N1—C9	179.6 (2)
C3—C2—C7—C8	−177.8 (2)	C14—C9—N1—C8	117.3 (3)
C1—C2—C7—C8	2.8 (2)	C10—C9—N1—C8	−60.2 (4)
C5—C6—C7—C2	−2.4 (3)	C14—C9—N1—C1	−59.9 (4)
Cl2—C6—C7—C2	176.82 (16)	C10—C9—N1—C1	122.7 (3)

Fig. 1

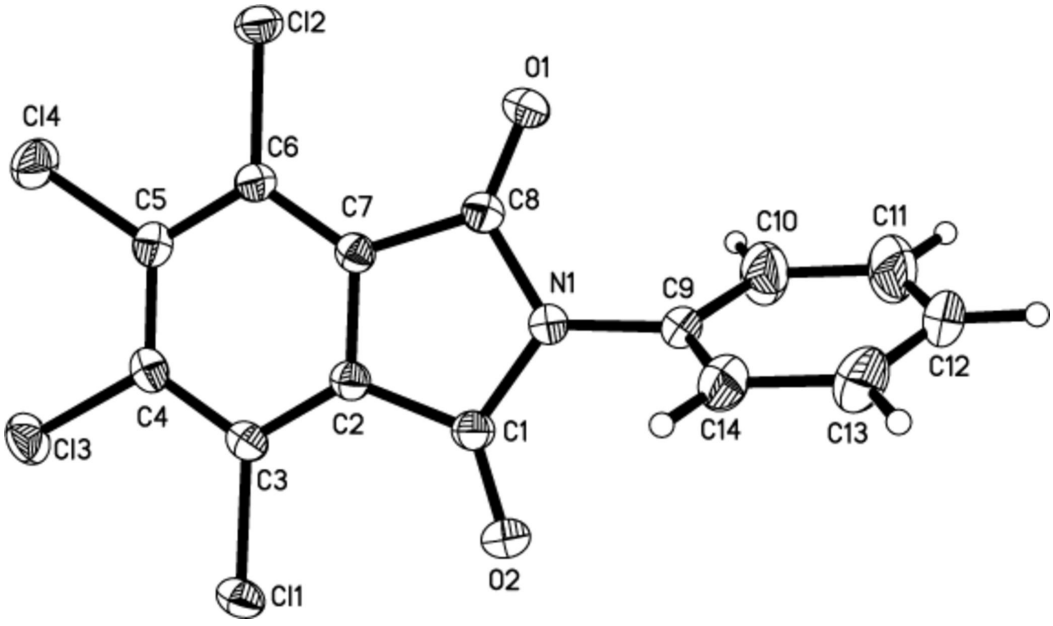
Cl2
O1
Cl4
C6
C5
C7
C8
C10
C11
N1
C9
C12
C4
C2
C1
C14
C13
Cl3
C3
O2
Cl1

Fig. 2