

3-(4-Butylphenylamino)isobenzofuran-1(3H)-one¹

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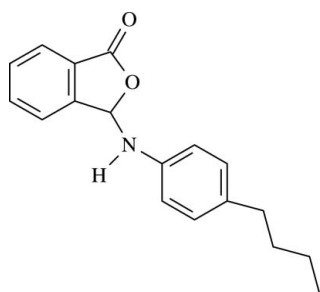
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.080; wR factor = 0.249; data-to-parameter ratio = 15.4.

The crystal structure of the title compound, $\text{C}_{18}\text{H}_{19}\text{NO}_2$, is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and also $\text{C}-\text{H}\cdots\pi$ interactions. These hydrogen-bond interactions generate edge-fused $R_2^2(8)R_2^2(10)-R_2^2(8)R_4^2(20)R_2^2(8)R_2^2(10)R_2^2(8)$ ring motifs. The phthalide group is planar and oriented at a dihedral angle of $57.92(16)^\circ$ with respect to the benzene ring.

Related literature

For related structures, see: Büyükgüngör & Odabaşoğlu (2006*a,b*, 2007); Odabaşoğlu & Büyükgüngör (2006*a,b,c,d,e,f,g,h,i,j,k,l,m,n,o,p,q,r*, 2007*a,cb,c,d,e,f*). For related literature, see: Aoki *et al.* (1973, 1974); Lacova (1973); Elderfield (1951); Tsi & Tan (1997). For general background, see: Etter (1990). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{19}\text{NO}_2$	$c = 18.875(2)$ Å
$M_r = 281.34$	$\alpha = 89.268(10)^\circ$
Triclinic, $P\bar{1}$	$\beta = 82.734(10)^\circ$
$a = 5.8603(7)$ Å	$\gamma = 76.045(10)^\circ$
$b = 7.2525(9)$ Å	$V = 772.18(16)$ Å ³

¹ 3-Substituted phthalides, Part XXIX. For Part XXVIII, see: Odabaşoğlu & Büyükgüngör (2007g).

$Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹

$T = 296$ K
 $0.71 \times 0.33 \times 0.07$ mm

Data collection

Stoe IPDS-2 diffractometer
Absorption correction: integration
(*X-RED32*; Stoe & Cie, 2002)
 $T_{\min} = 0.960$, $T_{\max} = 0.992$

16234 measured reflections
3002 independent reflections
1669 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.105$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.080$
 $wR(F^2) = 0.249$
 $S = 1.05$
3002 reflections
195 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.30$ e Å⁻³
 $\Delta\rho_{\min} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C1–C6 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H19}\cdots\text{O1}^{\text{i}}$	0.99 (4)	2.04 (4)	3.000 (4)	165 (3)
$\text{C3}-\text{H3}\cdots\text{O1}^{\text{ii}}$	0.93	2.44	3.331 (5)	161 (3)
$\text{C10}-\text{H10}\cdots\text{O2}^{\text{i}}$	0.93	2.70	3.450 (5)	139 (1)
$\text{C6}-\text{H6}\cdots\text{Cg1}^{\text{iii}}$	0.93	2.94 (3)	3.635 (4)	133 (1)
$\text{C17}-\text{H17B}\cdots\text{Cg1}^{\text{iv}}$	0.97	2.78 (3)	3.663 (6)	151 (1)

 Symmetry codes: (i) $x - 1, y, z$; (ii) $-x + 2, -y, -z + 1$; (iii) $x, y - 1, z$; (iv) $x, y + 1, z$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2339).

References

- Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.
- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Aoki, K., Furusho, T., Kimura, T., Satake, K. & Funayama, S. (1973). Jpn. Patent No. 7 324 724.
- Aoki, K., Furusho, T., Kimura, T., Satake, K. & Funayama, S. (1974). *Chem. Abstr.* **80**, 129246.
- Büyükgüngör, O. & Odabaşoğlu, M. (2006*a*). *Acta Cryst.* **E62**, o2003–o2004.
- Büyükgüngör, O. & Odabaşoğlu, M. (2006*b*). *Acta Cryst.* **E62**, o2936–o2937.
- Büyükgüngör, O. & Odabaşoğlu, M. (2007). *Acta Cryst.* **E63**, o25–o27.
- Elderfield, R. C. (1951). *Heterocyclic Compounds*, Vol. 2, ch. 2. New York: Wiley.
- Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Lacova, M. (1973). *Chem. Zvesti.* **27**, 525–535.
- Odabaşoğlu, M. & Büyükgüngör, O. (2006*a*). *Acta Cryst.* **E62**, o1879–o1881.
- Odabaşoğlu, M. & Büyükgüngör, O. (2006*b*). *Acta Cryst.* **E62**, o1882–o1883.
- Odabaşoğlu, M. & Büyükgüngör, O. (2006*c*). *Acta Cryst.* **E62**, o1884–o1885.

- Odabaşođlu, M. & Büyükgüngör, O. (2006*d*). *Acta Cryst.* **E62**, o2088–o2089.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*e*). *Acta Cryst.* **E62**, o2316–o2317.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*f*). *Acta Cryst.* **E62**, o2866–o2868.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*g*). *Acta Cryst.* **E62**, o2943–o2944.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*h*). *Acta Cryst.* **E62**, o4138–o4139.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*i*). *Acta Cryst.* **E62**, o2558–o2559.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*j*). *Acta Cryst.* **E62**, o3042–o3043.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*k*). *Acta Cryst.* **E62**, o2079–o2080.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*l*). *Acta Cryst.* **E62**, o2929–o2931.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*m*). *Acta Cryst.* **E62**, o4366–o4367.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*n*). *Acta Cryst.* **E62**, o4140–o4141.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*o*). *Acta Cryst.* **E62**, o4142–o4144.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*p*). *Acta Cryst.* **E62**, o4145–o4147.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*q*). *Acta Cryst.* **E62**, o4148–o4150.
- Odabaşođlu, M. & Büyükgüngör, O. (2006*r*). *Acta Cryst.* **E62**, o4151–o4153.
- Odabaşođlu, M. & Büyükgüngör, O. (2007*a*). *Acta Cryst.* **E63**, o22–o24.
- Odabaşođlu, M. & Büyükgüngör, O. (2007*b*). *Acta Cryst.* **E63**, o1999–o2001.
- Odabaşođlu, M. & Büyükgüngör, O. (2007*c*). *Acta Cryst.* **E63**, o2159–o2161.
- Odabaşođlu, M. & Büyükgüngör, O. (2007*d*). *Acta Cryst.* **E63**, o4296–o4297.
- Odabaşođlu, M. & Büyükgüngör, O. (2007*e*). *Acta Cryst.* **E63**, o4343.
- Odabaşođlu, M. & Büyükgüngör, O. (2007*f*). *Acta Cryst.* **E63**, o4348.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Tsi, D. & Tan, B. K. H. (1997). *Phytother. Res.* **11**, 576–582.

supplementary materials

Acta Cryst. (2007). E63, o4510-o4511 [doi:10.1107/S1600536807053226]

3-(4-Butylphenylamino)isobenzofuran-1(3H)-one

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Comment

Phthalides (isobenzofuranones) possess several important properties, such as fungicidal (Aoki *et al.*, 1973; Lacova, 1973), bactericidal and herbicidal (Lacova, 1973), analgesic (Elderfield, 1951), hypotensive and vasorelaxant activities (Tsi & Tan, 1997). Considering the potential interest of such phthalide-3-phosphonates in synthetic organic chemistry as agrochemical and pharmaceutical agents, we decided to investigate the solid-state structures of 3-substituted phthalides by *x*-ray diffraction methods. As part of a continuing study of the interplay between molecular conformation and supra-molecular aggregation in 3-substituted phthalides (Büyükgüngör & Odabaşođlu, 2006a,b; Odabaşođlu & Büyükgüngör, 2006a-r, 2007a-g), we report herein the structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The phthalide group (C1—C8/O2) is planar, the largest deviation from the mean plane being -0.026 (4) Å (for C6). The dihedral angle between the planar phthalide group and phenyl ring is 57.92 (16)°.

In (I), the crystal packing is stabilized by intermolecular N—H \cdots O and C—H \cdots O hydrogen bonds and also C—H \cdots π interactions (Table 1), which generate edge-fused $R_2^2(8)R_2^2(10)R_2^2(8)R_4^2(20)R_2^2(8)R_2^2(10)R_2^2(8)$ ring motifs (Fig. 2) (Etter, 1990). The hydrogen bonded motifs are linked to each other forming three-dimensional network (Fig. 3).

Experimental

The title compound, (I), was prepared according to the method described by Odabaşođlu & Büyükgüngör (2006a), using phthalaldehydic acid and 4-iodoaniline as starting materials (yield; 83%, m.p. 409–411 K). Crystals of (I) suitable for *x*-ray analysis were obtained by slow evaporation of a DMF solution at room temperature.

Refinement

H19 (for NH) was located in difference syntheses and refined isotropically [N—H = 0.99 (4) Å, $U_{\text{iso}}(\text{H}) = 0.066$ (11) Å²]. The remaining H atoms were positioned geometrically, with C—H = 0.93 , 0.98 , 0.97 and 0.96 Å, for aromatic, methine, methylene and methyl H atoms and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

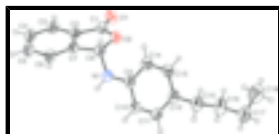


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

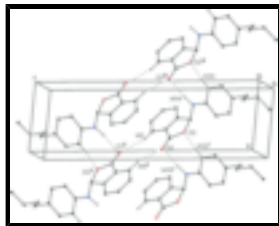


Fig. 2. A partial packing diagram of (I), showing the formation of $R_4^4(20)$ motif. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity [symmetry codes: (i) $x + 1, y, z$; (ii) $x + 1, -y, 1 - z$; (iii) $-x, y, z$].

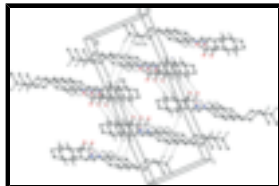


Fig. 3. A packing diagram of (I). Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

3-(4-Butylphenylamino)isobenzofuran-1(3H)-one

Crystal data

$C_{18}H_{19}NO_2$	$Z = 2$
$M_r = 281.34$	$F_{000} = 300$
Triclinic, $P\bar{1}$	$D_x = 1.210 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 5.8603 (7) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 7.2525 (9) \text{ \AA}$	Cell parameters from 16234 reflections
$c = 18.875 (2) \text{ \AA}$	$\theta = 2.2\text{--}27.3^\circ$
$\alpha = 89.268 (10)^\circ$	$\mu = 0.08 \text{ mm}^{-1}$
$\beta = 82.734 (10)^\circ$	$T = 296 \text{ K}$
$\gamma = 76.045 (10)^\circ$	Plane, colorless
$V = 772.18 (16) \text{ \AA}^3$	$0.71 \times 0.33 \times 0.07 \text{ mm}$

Data collection

Stoe IPDS-2 diffractometer	3002 independent reflections
Monochromator: plane graphite	1669 reflections with $I > 2\sigma(I)$
Detector resolution: $6.67 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.105$
$T = 296 \text{ K}$	$\theta_{\text{max}} = 26.0^\circ$
ω scans	$\theta_{\text{min}} = 2.2^\circ$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -7 \rightarrow 7$
$T_{\text{min}} = 0.960, T_{\text{max}} = 0.992$	$k = -8 \rightarrow 8$
16234 measured reflections	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of

	independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.080$	$w = 1/[\sigma^2(F_o^2) + (0.0977P)^2 + 0.5206P]$
$wR(F^2) = 0.249$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{\max} < 0.001$
3002 reflections	$\Delta\rho_{\max} = 0.30 \text{ e } \text{\AA}^{-3}$
195 parameters	$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.051 (11)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.9390 (5)	0.2237 (4)	0.41838 (16)	0.0799 (9)
O2	0.7034 (5)	0.2755 (4)	0.33295 (15)	0.0698 (8)
N1	0.3062 (6)	0.3156 (4)	0.30706 (19)	0.0642 (9)
H19	0.193 (7)	0.303 (5)	0.349 (2)	0.066 (11)*
C1	0.7958 (7)	0.1738 (5)	0.3882 (2)	0.0630 (10)
C2	0.6939 (7)	0.0084 (5)	0.3981 (2)	0.0603 (10)
C3	0.7386 (7)	-0.1397 (6)	0.4462 (2)	0.0673 (11)
H3	0.8495	-0.1452	0.4778	0.081*
C4	0.6142 (8)	-0.2759 (6)	0.4454 (2)	0.0734 (12)
H4	0.6401	-0.3757	0.4772	0.088*
C5	0.4506 (9)	-0.2681 (6)	0.3983 (3)	0.0791 (13)
H5	0.3711	-0.3646	0.3983	0.095*
C6	0.4009 (8)	-0.1202 (5)	0.3506 (2)	0.0702 (11)
H6	0.2865	-0.1136	0.3201	0.084*
C7	0.5296 (7)	0.0162 (5)	0.3507 (2)	0.0594 (10)
C8	0.5281 (7)	0.1874 (5)	0.3051 (2)	0.0621 (10)
H8	0.5860	0.1452	0.2556	0.074*
C9	0.2634 (7)	0.4695 (5)	0.2608 (2)	0.0601 (10)
C10	0.0367 (7)	0.5832 (5)	0.2629 (2)	0.0643 (10)
H10	-0.0839	0.5599	0.2962	0.077*
C11	-0.0127 (8)	0.7312 (5)	0.2161 (2)	0.0717 (11)

supplementary materials

H11	-0.1673	0.8049	0.2184	0.086*
C12	0.1583 (8)	0.7737 (6)	0.1661 (2)	0.0704 (11)
C13	0.3872 (8)	0.6597 (6)	0.1651 (2)	0.0781 (12)
H13	0.5071	0.6830	0.1316	0.094*
C14	0.4421 (7)	0.5127 (6)	0.2125 (2)	0.0717 (11)
H14	0.5980	0.4432	0.2120	0.086*
C15	0.1054 (10)	0.9338 (6)	0.1145 (3)	0.0890 (15)
H15A	0.2080	0.8983	0.0698	0.107*
H15B	-0.0571	0.9523	0.1047	0.107*
C16	0.1391 (12)	1.1171 (7)	0.1414 (3)	0.1084 (18)
H16A	0.3021	1.0979	0.1508	0.130*
H16B	0.0382	1.1507	0.1865	0.130*
C17	0.0844 (13)	1.2847 (8)	0.0908 (3)	0.116 (2)
H17A	-0.0642	1.2868	0.0728	0.139*
H17B	0.0636	1.4020	0.1176	0.139*
C18	0.2664 (14)	1.2782 (10)	0.0306 (4)	0.143 (3)
H18A	0.2871	1.1634	0.0033	0.171*
H18B	0.4130	1.2812	0.0477	0.171*
H18C	0.2198	1.3859	0.0010	0.171*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0755 (19)	0.091 (2)	0.085 (2)	-0.0365 (17)	-0.0207 (16)	0.0157 (16)
O2	0.0691 (17)	0.0628 (16)	0.0837 (19)	-0.0239 (13)	-0.0195 (14)	0.0228 (14)
N1	0.061 (2)	0.0579 (19)	0.071 (2)	-0.0118 (16)	-0.0050 (16)	0.0156 (16)
C1	0.062 (2)	0.058 (2)	0.068 (2)	-0.0150 (19)	-0.005 (2)	0.0097 (19)
C2	0.062 (2)	0.054 (2)	0.062 (2)	-0.0117 (17)	-0.0036 (18)	0.0065 (17)
C3	0.074 (3)	0.059 (2)	0.066 (2)	-0.010 (2)	-0.011 (2)	0.0105 (19)
C4	0.093 (3)	0.051 (2)	0.073 (3)	-0.015 (2)	-0.004 (2)	0.013 (2)
C5	0.100 (3)	0.051 (2)	0.087 (3)	-0.025 (2)	-0.004 (3)	0.003 (2)
C6	0.079 (3)	0.050 (2)	0.082 (3)	-0.016 (2)	-0.010 (2)	-0.006 (2)
C7	0.063 (2)	0.047 (2)	0.064 (2)	-0.0093 (17)	-0.0004 (18)	0.0009 (17)
C8	0.067 (2)	0.055 (2)	0.065 (2)	-0.0164 (19)	-0.0071 (19)	0.0053 (18)
C9	0.069 (2)	0.052 (2)	0.063 (2)	-0.0192 (18)	-0.0152 (19)	0.0112 (18)
C10	0.063 (2)	0.057 (2)	0.071 (3)	-0.0130 (19)	-0.0016 (19)	0.0022 (19)
C11	0.073 (3)	0.051 (2)	0.086 (3)	-0.0042 (19)	-0.014 (2)	0.005 (2)
C12	0.082 (3)	0.059 (2)	0.072 (3)	-0.019 (2)	-0.017 (2)	0.014 (2)
C13	0.082 (3)	0.080 (3)	0.074 (3)	-0.024 (2)	-0.005 (2)	0.023 (2)
C14	0.065 (2)	0.072 (3)	0.076 (3)	-0.016 (2)	-0.004 (2)	0.017 (2)
C15	0.115 (4)	0.068 (3)	0.089 (3)	-0.024 (3)	-0.030 (3)	0.019 (2)
C16	0.156 (5)	0.081 (3)	0.098 (4)	-0.038 (3)	-0.033 (4)	0.023 (3)
C17	0.148 (5)	0.079 (3)	0.116 (5)	-0.025 (4)	-0.013 (4)	0.024 (3)
C18	0.178 (7)	0.123 (5)	0.107 (5)	-0.017 (5)	0.015 (5)	0.022 (4)

Geometric parameters (\AA , $^\circ$)

N1—H19	0.99 (4)	C10—C11	1.381 (5)
C1—O1	1.197 (5)	C10—H10	0.9300

C1—O2	1.362 (5)	C11—C12	1.375 (6)
C1—C2	1.464 (5)	C11—H11	0.9300
C2—C7	1.386 (5)	C12—C13	1.394 (6)
C2—C3	1.395 (5)	C12—C15	1.506 (6)
C3—C4	1.363 (6)	C13—C14	1.387 (6)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.380 (6)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.495 (7)
C5—C6	1.391 (6)	C15—H15A	0.9700
C5—H5	0.9300	C15—H15B	0.9700
C6—C7	1.382 (5)	C16—C17	1.534 (7)
C6—H6	0.9300	C16—H16A	0.9700
C7—C8	1.501 (5)	C16—H16B	0.9700
C8—N1	1.400 (5)	C17—C18	1.449 (9)
C8—O2	1.484 (4)	C17—H17A	0.9700
C8—H8	0.9800	C17—H17B	0.9700
C9—C10	1.381 (5)	C18—H18A	0.9600
C9—C14	1.391 (5)	C18—H18B	0.9600
C9—N1	1.402 (5)	C18—H18C	0.9600
C1—O2—C8	110.5 (3)	C12—C11—C10	122.4 (4)
C8—N1—C9	122.6 (3)	C12—C11—H11	118.8
C8—N1—H19	114 (2)	C10—C11—H11	118.8
C9—N1—H19	122 (2)	C11—C12—C13	116.5 (4)
O1—C1—O2	120.5 (4)	C11—C12—C15	122.7 (4)
O1—C1—C2	131.3 (4)	C13—C12—C15	120.8 (4)
O2—C1—C2	108.2 (3)	C14—C13—C12	122.1 (4)
C7—C2—C3	121.2 (4)	C14—C13—H13	118.9
C7—C2—C1	109.2 (3)	C12—C13—H13	118.9
C3—C2—C1	129.6 (4)	C13—C14—C9	119.9 (4)
C4—C3—C2	117.8 (4)	C13—C14—H14	120.1
C4—C3—H3	121.1	C9—C14—H14	120.1
C2—C3—H3	121.1	C16—C15—C12	113.3 (4)
C3—C4—C5	121.0 (4)	C16—C15—H15A	108.9
C3—C4—H4	119.5	C12—C15—H15A	108.9
C5—C4—H4	119.5	C16—C15—H15B	108.9
C4—C5—C6	122.1 (4)	C12—C15—H15B	108.9
C4—C5—H5	119.0	H15A—C15—H15B	107.7
C6—C5—H5	119.0	C15—C16—C17	115.0 (5)
C7—C6—C5	116.8 (4)	C15—C16—H16A	108.5
C7—C6—H6	121.6	C17—C16—H16A	108.5
C5—C6—H6	121.6	C15—C16—H16B	108.5
C6—C7—C2	121.1 (3)	C17—C16—H16B	108.5
C6—C7—C8	130.7 (4)	H16A—C16—H16B	107.5
C2—C7—C8	108.3 (3)	C18—C17—C16	114.0 (6)
N1—C8—O2	111.7 (3)	C18—C17—H17A	108.8
N1—C8—C7	114.6 (3)	C16—C17—H17A	108.8
O2—C8—C7	103.7 (3)	C18—C17—H17B	108.8
N1—C8—H8	108.9	C16—C17—H17B	108.8
O2—C8—H8	108.9	H17A—C17—H17B	107.7

supplementary materials

C7—C8—H8	108.9	C17—C18—H18A	109.5
C10—C9—C14	118.3 (3)	C17—C18—H18B	109.5
C10—C9—N1	119.3 (3)	H18A—C18—H18B	109.5
C14—C9—N1	122.3 (4)	C17—C18—H18C	109.5
C11—C10—C9	120.6 (4)	H18A—C18—H18C	109.5
C11—C10—H10	119.7	H18B—C18—H18C	109.5
C9—C10—H10	119.7		
O1—C1—O2—C8	-179.2 (4)	N1—C8—O2—C1	123.2 (3)
C2—C1—O2—C8	2.3 (4)	C7—C8—O2—C1	-0.7 (4)
O1—C1—C2—C7	178.6 (4)	O2—C8—N1—C9	71.4 (4)
O2—C1—C2—C7	-3.1 (4)	C7—C8—N1—C9	-171.0 (3)
O1—C1—C2—C3	-0.4 (8)	C10—C9—N1—C8	176.1 (4)
O2—C1—C2—C3	177.9 (4)	C14—C9—N1—C8	-4.0 (6)
C7—C2—C3—C4	-0.4 (6)	C14—C9—C10—C11	2.7 (6)
C1—C2—C3—C4	178.6 (4)	N1—C9—C10—C11	-177.4 (4)
C2—C3—C4—C5	0.4 (6)	C10—C9—C14—C13	-3.9 (6)
C3—C4—C5—C6	-1.4 (7)	N1—C9—C14—C13	176.2 (4)
C4—C5—C6—C7	2.3 (6)	C9—C10—C11—C12	-0.5 (6)
C5—C6—C7—C2	-2.2 (6)	C10—C11—C12—C13	-0.4 (7)
C5—C6—C7—C8	177.3 (4)	C10—C11—C12—C15	179.5 (4)
C3—C2—C7—C6	1.4 (6)	C11—C12—C13—C14	-0.9 (7)
C1—C2—C7—C6	-177.8 (4)	C15—C12—C13—C14	179.2 (4)
C3—C2—C7—C8	-178.3 (4)	C12—C13—C14—C9	3.1 (7)
C1—C2—C7—C8	2.6 (4)	C11—C12—C15—C16	91.9 (6)
C6—C7—C8—N1	57.2 (6)	C13—C12—C15—C16	-88.3 (6)
C2—C7—C8—N1	-123.2 (4)	C12—C15—C16—C17	-179.3 (5)
C6—C7—C8—O2	179.2 (4)	C15—C16—C17—C18	-75.8 (8)
C2—C7—C8—O2	-1.2 (4)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H19 \cdots O1 ⁱ	0.99 (4)	2.04 (4)	3.000 (4)	165 (3)
C3—H3 \cdots O1 ⁱⁱ	0.93	2.44	3.331 (5)	161 (3)
C10—H10 \cdots O2 ⁱ	0.93	2.70	3.450 (5)	139 (1)
C6—H6 \cdots Cg1 ⁱⁱⁱ	0.93	2.94 (3)	3.635 (4)	133 (1)
C17—H17B \cdots Cg1 ^{iv}	0.97	2.78 (3)	3.663 (6)	151 (1)

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y, -z+1$; (iii) $x, y-1, z$; (iv) $x, y+1, z$.

Fig. 1

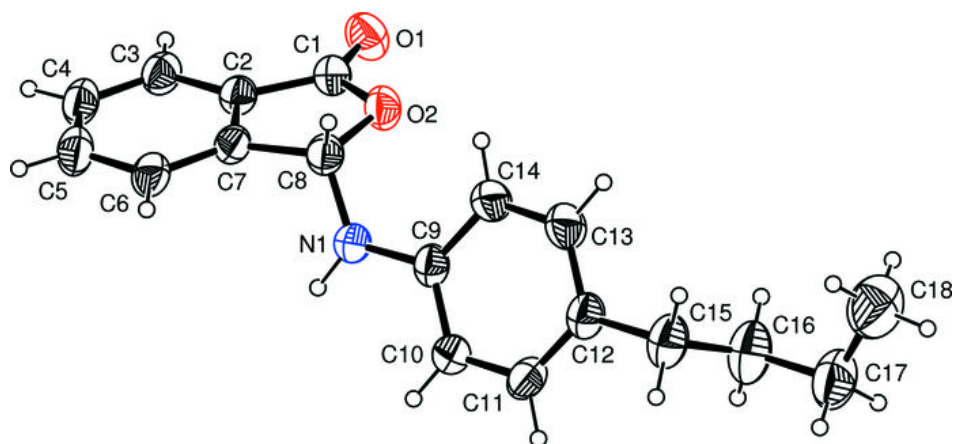


Fig. 2

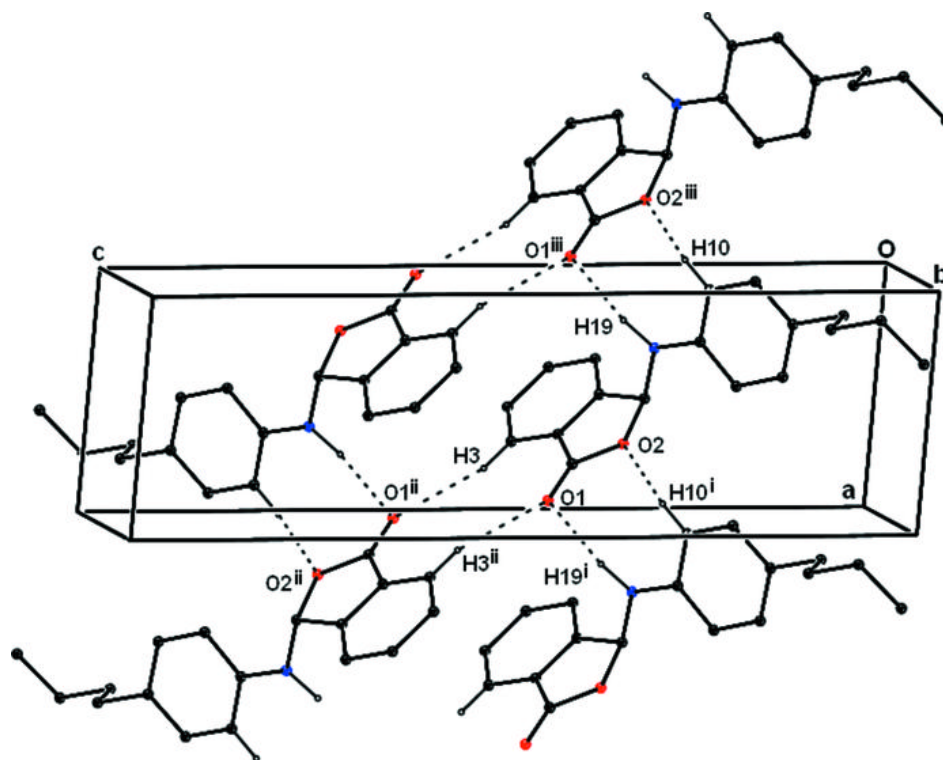


Fig. 3

