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N,*N*′-(Oxydi-*p*-phenylene)diphthalimide

Yi-Tao Li[a]* and Zhiguo Wang[b]

[a]Key Laboratory of Pesticides and Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China, and [b]School of Chemical and Materials Engineering, Huangshi Institute of Technology, Huangshi 435003, People's Republic of China
Correspondence e-mail: lytm1234@yahoo.com.cn

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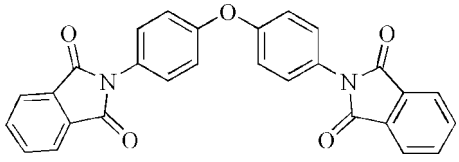
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.004 Å; R factor = 0.046; wR factor = 0.118; data-to-parameter ratio = 9.3.

The title compound, $C_{28}H_{16}N_2O_5$, is a bis-imide derivative in which two phthalimide units are linked by an oxydi-*p*-phenylene bridge. The dihedral angle between the planes of the two central benzene rings is 86.1 (4)°. The isoindole groups make dihedral angles of 46.0 (14) and 77.5 (13)° with the attached benzene rings. Intermolecular C—H···O hydrogen bonds contribute to the stability of the structure.

Related literature

For details of the biological activity and uses of bis-imide derivatives, see: Rich *et al.* (1975); Degenhardt *et al.* (2002); Mallakpour & Kowsari (2004); Zhang *et al.* (1999); Langhals & Kirner (2000); Yakimov & Forrest (2002). For a related structure, see: Li *et al.* (2007).



Experimental

Crystal data

$C_{28}H_{16}N_2O_5$
M_r = 460.43
Orthorhombic, $P2_12_12_1$
a = 7.5059 (11) Å
b = 16.480 (3) Å
c = 17.551 (3) Å
V = 2171.0 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 292 (2) K
0.30 × 0.30 × 0.30 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
13091 measured reflections
2925 independent reflections
2644 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.118
S = 1.23
2925 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···O5^{i}	0.93	2.47	3.222 (4)	138
C19—H19···O5^{ii}	0.93	2.56	3.298 (4)	136

Symmetry codes: (i) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+2$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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*.

The authors thank Dr Xiang-Gao Meng for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2220).

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supplementary materials

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N,*N*'-(Oxydi-*p*-phenylene)diphthalimide

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Comment

Bisimides are heterocyclic compounds, some of which have biological activity (Rich *et al.*, 1975). Moreover, they are synthetic precursors with applications in organic synthesis (Degenhardt *et al.*, 2002), polymer synthesis (Mallakpour & Kowsari, 2004), supramolecular chemistry (Zhang *et al.*, 1999), and for the development of new materials (Langhals & Kirner, 2000) and molecular electronic devices (Yakimov & Forrest, 2002).

Following our studies on the synthesis of bisimide derivatives (Li *et al.*, 2007), we report here the structure of the title compound (Fig. 1). The two phthalimide units are linked by a (phenoxy)phenylene bridge. The dihedral angle between the planes of the two central benzene rings is 86.1 (4)° The isoindole groups make dihedral angles of 46.0 (14)° and 77.5 (13)° with the attached benzene rings. Compared to a similar structure, *N*,*N*'-(methylenedi-*p*-phenylene)diphthalimide (Li *et al.*, 2007), the packing pattern is different; this may be due to the bridging methylene group being replaced by the bridging O atom. Intermolecular C—H···O hydrogen bonds contribute to the stability of the structure (Table 1).

Experimental

A solution of phthaloyl dichoride (420 mg, 2 mmol) was added slowly over a period of 10 min to a solution of 4-aminophenyl ether (400 mg, 2 mmol) in dichloromethane (25 ml) at 273 K to yield a light yellow precipitate. Triethylamine (5 ml) was then added to dissolve the precipitate which became a yellow suspension after stirring for 12 h. The compound was filtered and dried (yield 510 mg, 70%). Single crystals of the title compound were obtained by recrystallization from dimethylformamide at room temperature.

Refinement

All H atoms were initially located in a difference Fourier map; they were then placed in calculated positions and constrained to ride on their parent atoms, with C—-H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Figures

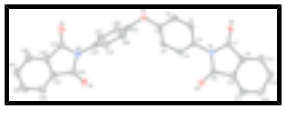


Fig. 1. The molecular structure of the title compound, with 50% probability displacement ellipsoids. H atoms have been omitted.

N,*N*'-(Oxydi-*p*-phenylene)diphthalimide

Crystal data

$C_{28}H_{16}N_2O_5$	F_{000} = 952
M_r = 460.43	D_x = 1.409 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 5562 reflections
a = 7.5059 (11) Å	θ = 2.3–25.9º
b = 16.480 (3) Å	μ = 0.10 mm^{-1}
c = 17.551 (3) Å	T = 292 (2) K
V = 2171.0 (6) Å^3	Block, colourless
Z = 4	0.30 × 0.30 × 0.30 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer	2644 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.027
Monochromator: graphite	θ_{max} = 28.0º
T = 292(2) K	θ_{min} = 2.3º
φ and ω scans	h = −8→9
Absorption correction: none	k = −21→17
13091 measured reflections	l = −22→22
2925 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 0.1294P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.046	$(\Delta/\sigma)_{max}$ = 0.017
$wR(F^2)$ = 0.118	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
S = 1.23	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
2925 reflections	Extinction correction: none
316 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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	0.8558 (3)	0.62700 (13)	1.04648 (13)	0.0449 (5)
C2	0.9322 (4)	0.70185 (14)	1.05712 (13)	0.0492 (5)
H2	0.9588	0.7202	1.1059	0.059*
C3	0.9691 (4)	0.74958 (14)	0.99444 (15)	0.0492 (6)
H3	1.0231	0.7999	1.0009	0.059*
C4	0.9259 (3)	0.72283 (12)	0.92192 (12)	0.0432 (5)
C5	0.8447 (4)	0.64854 (13)	0.91224 (12)	0.0474 (5)
H5	0.8124	0.6313	0.8637	0.057*
C6	0.8115 (4)	0.59984 (13)	0.97454 (13)	0.0485 (5)
H6	0.7595	0.5491	0.9681	0.058*
C7	0.9251 (4)	0.85440 (13)	0.84975 (13)	0.0474 (5)
C8	1.0414 (4)	0.74006 (15)	0.78915 (14)	0.0506 (6)
C9	0.9801 (3)	0.87704 (15)	0.77128 (14)	0.0491 (5)
C10	1.0480 (3)	0.80952 (15)	0.73544 (13)	0.0494 (5)
C11	1.1046 (4)	0.81216 (19)	0.66035 (15)	0.0616 (7)
H11	1.1511	0.7665	0.6363	0.074*
C12	1.0891 (5)	0.8850 (2)	0.62283 (15)	0.0712 (9)
H12	1.1250	0.8886	0.5722	0.085*
C13	1.0219 (4)	0.9526 (2)	0.65846 (17)	0.0706 (9)
H13	1.0131	1.0009	0.6313	0.085*
C14	0.9667 (4)	0.95066 (17)	0.73407 (16)	0.0598 (7)
H14	0.9228	0.9966	0.7584	0.072*
C15	0.8345 (4)	0.49870 (14)	1.10677 (13)	0.0493 (6)
C16	0.6860 (4)	0.45102 (17)	1.11019 (18)	0.0634 (7)
H16	0.5730	0.4742	1.1105	0.076*
C17	0.7065 (4)	0.36759 (17)	1.11325 (19)	0.0649 (7)
H17	0.6066	0.3343	1.1156	0.078*
C18	0.8727 (4)	0.33395 (13)	1.11278 (13)	0.0484 (6)
C19	1.0208 (4)	0.38264 (17)	1.1071 (2)	0.0687 (8)
H19	1.1340	0.3598	1.1052	0.082*
C20	0.9999 (4)	0.46591 (17)	1.1043 (2)	0.0693 (8)
H20	1.0993	0.4994	1.1006	0.083*
C21	0.9359 (4)	0.20766 (15)	1.18659 (14)	0.0559 (6)

C22	0.8648 (4)	0.19351 (15)	1.05848 (15)	0.0577 (7)
C23	0.9404 (4)	0.12045 (15)	1.16640 (15)	0.0556 (6)
C24	0.8952 (4)	0.11189 (15)	1.09096 (15)	0.0563 (6)
C25	0.8777 (5)	0.03623 (17)	1.0583 (2)	0.0741 (9)
H25	0.8460	0.0300	1.0074	0.089*
C26	0.9095 (6)	−0.03000 (18)	1.1046 (3)	0.0897 (12)
H26	0.8972	−0.0819	1.0844	0.108*
C27	0.9587 (6)	−0.0216 (2)	1.1793 (3)	0.0890 (12)
H27	0.9808	−0.0676	1.2085	0.107*
C28	0.9758 (5)	0.05402 (19)	1.2116 (2)	0.0757 (9)
H28	1.0101	0.0601	1.2622	0.091*
N1	0.9654 (3)	0.77149 (11)	0.85670 (10)	0.0471 (5)
N2	0.8933 (3)	0.24810 (11)	1.11843 (11)	0.0533 (5)
O1	0.8144 (3)	0.58251 (10)	1.11128 (10)	0.0597 (5)
O2	0.8594 (3)	0.89603 (10)	0.89869 (11)	0.0626 (5)
O3	1.0881 (3)	0.67169 (11)	0.77944 (11)	0.0703 (6)
O4	0.9586 (4)	0.24056 (13)	1.24656 (11)	0.0848 (8)
O5	0.8234 (4)	0.21334 (12)	0.99506 (11)	0.0835 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0544 (13)	0.0353 (10)	0.0449 (11)	0.0030 (10)	0.0066 (10)	0.0026 (9)
C2	0.0603 (14)	0.0456 (12)	0.0416 (10)	−0.0062 (11)	−0.0017 (11)	−0.0034 (9)
C3	0.0631 (15)	0.0353 (9)	0.0491 (11)	−0.0105 (10)	−0.0011 (11)	−0.0034 (9)
C4	0.0522 (12)	0.0335 (9)	0.0437 (10)	0.0012 (9)	0.0038 (10)	0.0009 (9)
C5	0.0631 (14)	0.0363 (11)	0.0427 (11)	0.0000 (10)	−0.0001 (11)	−0.0062 (9)
C6	0.0644 (14)	0.0298 (9)	0.0515 (12)	−0.0061 (10)	0.0062 (11)	−0.0041 (9)
C7	0.0549 (13)	0.0344 (10)	0.0528 (13)	−0.0017 (10)	0.0010 (11)	0.0026 (9)
C8	0.0596 (15)	0.0459 (13)	0.0464 (12)	−0.0013 (11)	0.0034 (11)	−0.0033 (10)
C9	0.0511 (13)	0.0459 (12)	0.0502 (12)	−0.0065 (10)	−0.0071 (11)	0.0058 (10)
C10	0.0522 (13)	0.0511 (13)	0.0449 (12)	−0.0085 (11)	−0.0035 (10)	0.0019 (10)
C11	0.0655 (17)	0.0728 (17)	0.0467 (12)	−0.0166 (14)	−0.0006 (12)	−0.0007 (12)
C12	0.0768 (19)	0.090 (2)	0.0469 (13)	−0.0275 (18)	−0.0038 (13)	0.0141 (15)
C13	0.0731 (19)	0.0712 (18)	0.0674 (17)	−0.0239 (16)	−0.0144 (15)	0.0306 (16)
C14	0.0633 (16)	0.0489 (13)	0.0673 (16)	−0.0089 (12)	−0.0110 (14)	0.0154 (12)
C15	0.0711 (16)	0.0379 (11)	0.0387 (10)	−0.0051 (11)	0.0079 (11)	0.0024 (9)
C16	0.0620 (16)	0.0486 (13)	0.0797 (18)	0.0008 (12)	−0.0009 (15)	0.0064 (13)
C17	0.0617 (16)	0.0456 (13)	0.087 (2)	−0.0137 (12)	0.0021 (15)	0.0080 (14)
C18	0.0660 (15)	0.0370 (10)	0.0423 (11)	−0.0051 (11)	0.0033 (11)	0.0042 (9)
C19	0.0567 (15)	0.0478 (14)	0.102 (2)	−0.0010 (12)	0.0124 (16)	−0.0028 (15)
C20	0.0626 (17)	0.0446 (13)	0.101 (2)	−0.0120 (13)	0.0191 (16)	−0.0048 (15)
C21	0.0687 (17)	0.0492 (14)	0.0496 (13)	−0.0032 (13)	0.0003 (12)	0.0084 (11)
C22	0.0773 (18)	0.0470 (13)	0.0489 (13)	−0.0085 (13)	0.0083 (13)	−0.0022 (10)
C23	0.0586 (14)	0.0461 (12)	0.0622 (14)	0.0027 (12)	0.0086 (12)	0.0093 (11)
C24	0.0628 (15)	0.0429 (12)	0.0633 (14)	−0.0016 (11)	0.0173 (13)	−0.0003 (11)
C25	0.088 (2)	0.0525 (15)	0.0818 (19)	−0.0029 (16)	0.0251 (18)	−0.0115 (15)
C26	0.099 (3)	0.0418 (14)	0.128 (3)	0.0071 (16)	0.044 (3)	−0.0095 (18)

C27	0.094 (3)	0.0545 (17)	0.118 (3)	0.0193 (18)	0.030 (2)	0.0254 (19)
C28	0.083 (2)	0.0565 (17)	0.088 (2)	0.0114 (15)	0.0092 (18)	0.0242 (16)
N1	0.0628 (12)	0.0349 (9)	0.0436 (9)	−0.0002 (9)	0.0033 (9)	0.0016 (8)
N2	0.0771 (14)	0.0392 (9)	0.0437 (10)	−0.0040 (10)	−0.0006 (10)	0.0045 (8)
O1	0.0951 (14)	0.0372 (8)	0.0470 (9)	−0.0010 (9)	0.0187 (10)	0.0013 (7)
O2	0.0824 (13)	0.0389 (9)	0.0666 (11)	0.0050 (9)	0.0175 (10)	−0.0008 (8)
O3	0.1010 (15)	0.0449 (9)	0.0649 (10)	0.0095 (10)	0.0192 (12)	−0.0044 (8)
O4	0.138 (2)	0.0649 (12)	0.0520 (11)	−0.0018 (14)	−0.0199 (13)	0.0008 (9)
O5	0.142 (2)	0.0636 (12)	0.0452 (10)	−0.0148 (14)	−0.0081 (12)	0.0031 (9)

Geometric parameters (Å, °)

C1—C2	1.373 (3)	C15—C20	1.354 (4)
C1—C6	1.380 (3)	C15—C16	1.365 (4)
C1—O1	1.388 (3)	C15—O1	1.392 (3)
C2—C3	1.380 (3)	C16—C17	1.385 (4)
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.385 (3)	C17—C18	1.365 (4)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.378 (3)	C18—C19	1.374 (4)
C4—N1	1.429 (3)	C18—N2	1.427 (3)
C5—C6	1.379 (3)	C19—C20	1.382 (4)
C5—H5	0.9300	C19—H19	0.9300
C6—H6	0.9300	C20—H20	0.9300
C7—O2	1.205 (3)	C21—O4	1.196 (3)
C7—N1	1.405 (3)	C21—N2	1.406 (3)
C7—C9	1.485 (3)	C21—C23	1.481 (4)
C8—O3	1.192 (3)	C22—O5	1.201 (3)
C8—N1	1.414 (3)	C22—N2	1.401 (3)
C8—C10	1.484 (3)	C22—C24	1.478 (4)
C9—C10	1.376 (4)	C23—C24	1.374 (4)
C9—C14	1.382 (3)	C23—C28	1.378 (4)
C10—C11	1.385 (4)	C24—C25	1.378 (4)
C11—C12	1.374 (4)	C25—C26	1.381 (5)
C11—H11	0.9300	C25—H25	0.9300
C12—C13	1.374 (5)	C26—C27	1.368 (6)
C12—H12	0.9300	C26—H26	0.9300
C13—C14	1.391 (4)	C27—C28	1.375 (5)
C13—H13	0.9300	C27—H27	0.9300
C14—H14	0.9300	C28—H28	0.9300
C2—C1—C6	121.1 (2)	C15—C16—H16	120.6
C2—C1—O1	117.2 (2)	C17—C16—H16	120.6
C6—C1—O1	121.6 (2)	C18—C17—C16	120.3 (3)
C1—C2—C3	119.2 (2)	C18—C17—H17	119.8
C1—C2—H2	120.4	C16—C17—H17	119.8
C3—C2—H2	120.4	C17—C18—C19	120.2 (2)
C2—C3—C4	120.3 (2)	C17—C18—N2	120.1 (2)
C2—C3—H3	119.9	C19—C18—N2	119.8 (3)
C4—C3—H3	119.9	C18—C19—C20	119.4 (3)

C5—C4—C3	120.0 (2)	C18—C19—H19	120.3
C5—C4—N1	119.44 (19)	C20—C19—H19	120.3
C3—C4—N1	120.60 (19)	C15—C20—C19	119.9 (3)
C4—C5—C6	119.9 (2)	C15—C20—H20	120.0
C4—C5—H5	120.0	C19—C20—H20	120.0
C6—C5—H5	120.0	O4—C21—N2	124.5 (2)
C1—C6—C5	119.5 (2)	O4—C21—C23	130.3 (2)
C1—C6—H6	120.2	N2—C21—C23	105.2 (2)
C5—C6—H6	120.2	O5—C22—N2	124.1 (2)
O2—C7—N1	125.5 (2)	O5—C22—C24	130.1 (2)
O2—C7—C9	129.2 (2)	N2—C22—C24	105.7 (2)
N1—C7—C9	105.4 (2)	C24—C23—C28	121.4 (3)
O3—C8—N1	125.8 (2)	C24—C23—C21	108.9 (2)
O3—C8—C10	128.9 (2)	C28—C23—C21	129.6 (3)
N1—C8—C10	105.29 (19)	C23—C24—C25	121.1 (3)
C10—C9—C14	121.4 (2)	C23—C24—C22	108.4 (2)
C10—C9—C7	108.9 (2)	C25—C24—C22	130.4 (3)
C14—C9—C7	129.7 (3)	C24—C25—C26	117.0 (3)
C9—C10—C11	121.5 (2)	C24—C25—H25	121.5
C9—C10—C8	108.7 (2)	C26—C25—H25	121.5
C11—C10—C8	129.7 (2)	C27—C26—C25	122.0 (3)
C12—C11—C10	117.2 (3)	C27—C26—H26	119.0
C12—C11—H11	121.4	C25—C26—H26	119.0
C10—C11—H11	121.4	C26—C27—C28	120.8 (3)
C11—C12—C13	121.4 (3)	C26—C27—H27	119.6
C11—C12—H12	119.3	C28—C27—H27	119.6
C13—C12—H12	119.3	C27—C28—C23	117.6 (3)
C12—C13—C14	121.6 (3)	C27—C28—H28	121.2
C12—C13—H13	119.2	C23—C28—H28	121.2
C14—C13—H13	119.2	C7—N1—C8	111.74 (19)
C9—C14—C13	116.7 (3)	C7—N1—C4	124.81 (19)
C9—C14—H14	121.6	C8—N1—C4	123.36 (18)
C13—C14—H14	121.6	C22—N2—C21	111.7 (2)
C20—C15—C16	121.3 (2)	C22—N2—C18	124.6 (2)
C20—C15—O1	119.8 (2)	C21—N2—C18	123.6 (2)
C16—C15—O1	118.7 (3)	C1—O1—C15	116.95 (18)
C15—C16—C17	118.8 (3)		
C6—C1—C2—C3	−1.7 (4)	C28—C23—C24—C25	2.2 (5)
O1—C1—C2—C3	−177.4 (2)	C21—C23—C24—C25	−175.8 (3)
C1—C2—C3—C4	1.4 (4)	C28—C23—C24—C22	179.7 (3)
C2—C3—C4—C5	0.5 (4)	C21—C23—C24—C22	1.7 (3)
C2—C3—C4—N1	−179.3 (2)	O5—C22—C24—C23	−180.0 (3)
C3—C4—C5—C6	−2.0 (4)	N2—C22—C24—C23	−0.4 (3)
N1—C4—C5—C6	177.8 (2)	O5—C22—C24—C25	−2.8 (6)
C2—C1—C6—C5	0.2 (4)	N2—C22—C24—C25	176.8 (3)
O1—C1—C6—C5	175.7 (2)	C23—C24—C25—C26	−0.7 (5)
C4—C5—C6—C1	1.7 (4)	C22—C24—C25—C26	−177.6 (4)
O2—C7—C9—C10	−179.7 (3)	C24—C25—C26—C27	−0.9 (6)
N1—C7—C9—C10	0.2 (3)	C25—C26—C27—C28	1.0 (6)

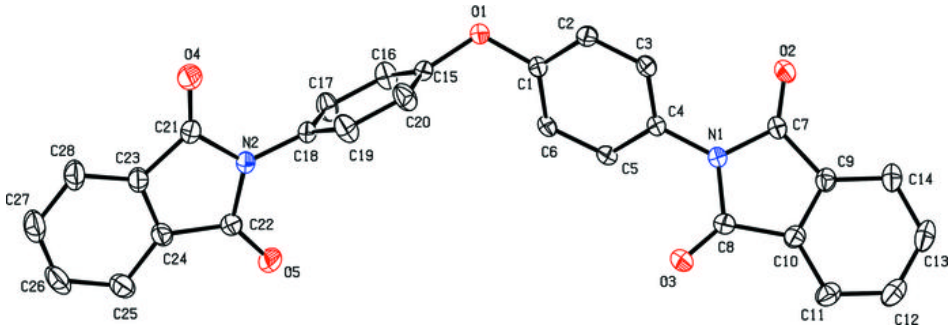
O2—C7—C9—C14	−1.5 (5)	C26—C27—C28—C23	0.5 (6)
N1—C7—C9—C14	178.4 (3)	C24—C23—C28—C27	−2.1 (5)
C14—C9—C10—C11	−0.5 (4)	C21—C23—C28—C27	175.5 (3)
C7—C9—C10—C11	177.8 (2)	O2—C7—N1—C8	179.9 (3)
C14—C9—C10—C8	−178.7 (2)	C9—C7—N1—C8	0.1 (3)
C7—C9—C10—C8	−0.4 (3)	O2—C7—N1—C4	3.4 (4)
O3—C8—C10—C9	−179.8 (3)	C9—C7—N1—C4	−176.5 (2)
N1—C8—C10—C9	0.4 (3)	O3—C8—N1—C7	179.9 (3)
O3—C8—C10—C11	2.2 (5)	C10—C8—N1—C7	−0.3 (3)
N1—C8—C10—C11	−177.6 (3)	O3—C8—N1—C4	−3.4 (4)
C9—C10—C11—C12	−0.4 (4)	C10—C8—N1—C4	176.4 (2)
C8—C10—C11—C12	177.4 (3)	C5—C4—N1—C7	131.9 (3)
C10—C11—C12—C13	0.6 (5)	C3—C4—N1—C7	−48.3 (4)
C11—C12—C13—C14	0.1 (5)	C5—C4—N1—C8	−44.3 (3)
C10—C9—C14—C13	1.2 (4)	C3—C4—N1—C8	135.5 (3)
C7—C9—C14—C13	−176.8 (3)	O5—C22—N2—C21	178.5 (3)
C12—C13—C14—C9	−1.0 (4)	C24—C22—N2—C21	−1.1 (3)
C20—C15—C16—C17	1.8 (4)	O5—C22—N2—C18	1.6 (5)
O1—C15—C16—C17	−173.8 (3)	C24—C22—N2—C18	−178.0 (3)
C15—C16—C17—C18	0.0 (5)	O4—C21—N2—C22	−176.6 (3)
C16—C17—C18—C19	−1.8 (4)	C23—C21—N2—C22	2.1 (3)
C16—C17—C18—N2	178.0 (3)	O4—C21—N2—C18	0.3 (5)
C17—C18—C19—C20	2.0 (5)	C23—C21—N2—C18	179.0 (3)
N2—C18—C19—C20	−177.8 (3)	C17—C18—N2—C22	77.1 (4)
C16—C15—C20—C19	−1.7 (5)	C19—C18—N2—C22	−103.1 (3)
O1—C15—C20—C19	173.8 (3)	C17—C18—N2—C21	−99.4 (3)
C18—C19—C20—C15	−0.2 (5)	C19—C18—N2—C21	80.4 (4)
O4—C21—C23—C24	176.3 (4)	C2—C1—O1—C15	−144.7 (3)
N2—C21—C23—C24	−2.3 (3)	C6—C1—O1—C15	39.6 (4)
O4—C21—C23—C28	−1.5 (6)	C20—C15—O1—C1	71.4 (3)
N2—C21—C23—C28	179.9 (3)	C16—C15—O1—C1	−113.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O5^{i}	0.93	2.47	3.222 (4)	138
C19—H19···O5^{ii}	0.93	2.56	3.298 (4)	136

Symmetry codes: (i) −*x*+2, *y*+1/2, −*z*+3/2; (ii) *x*+1/2, −*y*+1/2, −*z*+2.

Fig. 1


O1
C2
C3
O2
O4
C16
C15
C1
C17
C4
C7
C21
N2
C18
C19
C20
C6
C5
N1
C9
C14
C28
C23
C27
C22
C8
C10
C13
C24
O5
O3
C26
C25
C11
C12