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

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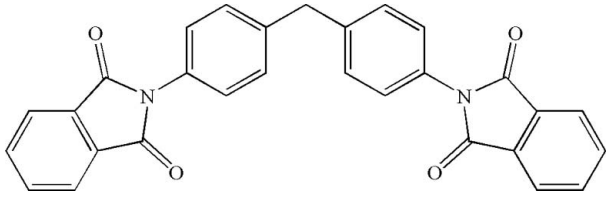
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; R factor = 0.050; wR factor = 0.135; data-to-parameter ratio = 8.9.

The title compound, $C_{29}H_{18}N_2O_4$, crystallizes with one half-molecule in the asymmetric unit, the other half being generated by a crystallographic twofold rotation axis passing through the central C atom. The dihedral angle between the planes of the two central benzene rings is 67.7 (4)°. The terminal isoindole group is approximately planar and makes a dihedral angle of 39.20 (17)° with the attached benzene ring. Intermolecular C—H···O hydrogen bonds contribute to the stability of the structure.

Related literature

For general background regarding diphthalimide, see: Guzmán-Lucero *et al.* (2006).



Experimental

Crystal data

$C_{29}H_{18}N_2O_4$
M_r = 458.45
Monoclinic, $C2$
a = 31.669 (6) Å
b = 4.913 (1) Å
c = 7.1543 (14) Å
β = 101.087 (3)°
V = 1092.4 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 292 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4 K CCD area-detector diffractometer
Absorption correction: none
4646 measured reflections
1414 independent reflections
1161 reflections with $I > 2\sigma(I)$
R_{int} = 0.099

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.136
S = 1.05
1414 reflections
159 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1^{i}	0.93	2.57	3.251 (4)	131

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

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: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

The authors thank Professor An-Xin Wu for technical assistance and Dr Xiang-Gao Meng for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WK2067).

References

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supplementary materials

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

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Comment

Bisimides are heterocyclic compounds, of which some have biological activivity. Moreover, they are synthetic precursor with application in organic synthesis, supramolecular chemistry, polymer synthesis, and for the development new materials and molecular electronic devices (Guzmán-Lucero *et al.*, 2006).

The molecule of the title, (I) is shown in Fig. 1. The compound crystallizes with one half-molecule in the asymmetric unit, the other half being generated by a crystallographic twofold rotation axis passing through the central C atom. There are no signicant different between the bonds and angles of the two molecules. The dihedral angle between the planes of the two central benzene rings is 67.7 (4)°. The terminal isoindole group is approximately planar and makes adihedral angle of 39.20 (17)° with the attached benzene ring.

Intermolecular C—H···O hydrogen bonds contribute to the stability of the structure (Table 1).

Experimental

A solution of phthaloyl dichoride (420, 2 mmol) was added slowly over a period of 10 min to a solution of 4-(4-aminobenzyl)benzenamine (240 mg, 2 mmol) in dichloromethane (20 ml) at 273 K with light yellow solid precipitated. Triethylamine (5 ml) was then added, while the pecipitated light yellow solid was dissolved. After being stirred for 10 hr,the reacted solution became yellow suspension·The compound was purified by filtration with suction and dried (I) (yield 410 mg, 29.14%). Single crystals of (I) were obtained by recrystallization from DMF at room temperature.

Refinement

All H atoms were initially located in a difference Fourier map and then included with constrained bond lengths and isotropic displacement parameters: C—H=0.93Å and U_{iso}(H)=1.5U_{eq}(C) for methyl, C—H=0.97Å and U_{iso}(H)=1.2U_{eq}(C) for methylene.

Figures

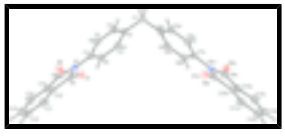


Fig. 1. The molecular structure of (I) with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

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

Crystal data

$C_{29}H_{18}N_2O_4$	F_{000} = 476
M_r = 458.45	D_x = 1.394 Mg m^{-3}
Monoclinic, *C*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C 2y	Cell parameters from 1420 reflections
a = 31.669 (6) Å	θ = 2.6–23.9º
b = 4.913 (1) Å	μ = 0.09 mm^{-1}
c = 7.1543 (14) Å	*T* = 292 (2) K
β = 101.087 (3)º	Plate, colorless
V = 1092.4 (4) Å^3	0.30 × 0.20 × 0.20 mm
Z = 2	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	1161 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.099
Monochromator: graphite	θ_{max} = 27.7º
T = 292(2) K	θ_{min} = 1.3º
φ and ω scans	*h* = −38→40
Absorption correction: none	*k* = −6→6
4646 measured reflections	*l* = −9→9
1414 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.050	$w = 1/[\sigma^2(F_o^2) + (0.0709P)^2 + 0.0873P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.136	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.05	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
1414 reflections	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
159 parameters	Extinction correction: none
1 restraint	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

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}	Occ. (<1)
C1	0.0000	1.2197 (11)	0.5000	0.0462 (11)	
H1A	0.0149	1.3359	0.4244	0.055*	0.50
H1B	−0.0149	1.3359	0.5756	0.055*	0.50
O1	0.08076 (7)	0.4639 (6)	1.2283 (3)	0.0545 (6)	
N1	0.12141 (7)	0.5510 (6)	0.9965 (3)	0.0411 (6)	
C2	0.03274 (8)	1.0474 (6)	0.6323 (4)	0.0380 (7)	
C6	0.08665 (9)	0.6935 (7)	0.6772 (4)	0.0430 (8)	
H6	0.1027	0.5654	0.6253	0.052*	
C7	0.09194 (9)	0.7230 (7)	0.8729 (4)	0.0382 (7)	
C5	0.06775 (10)	0.9128 (7)	0.9478 (4)	0.0453 (8)	
H5	0.0711	0.9328	1.0791	0.054*	
C8	0.11301 (9)	0.4301 (7)	1.1647 (4)	0.0411 (7)	
C3	0.03847 (10)	1.0736 (7)	0.8271 (4)	0.0462 (8)	
H3	0.0224	1.2017	0.8788	0.055*	
C4	0.05731 (9)	0.8558 (7)	0.5600 (4)	0.0433 (7)	
H4	0.0540	0.8359	0.4287	0.052*	
C10	0.15041 (9)	0.2547 (7)	1.2393 (4)	0.0436 (7)	
C9	0.16170 (9)	0.4632 (8)	0.9611 (4)	0.0467 (8)	
C15	0.17918 (9)	0.2712 (7)	1.1170 (4)	0.0452 (8)	
O2	0.17754 (7)	0.5373 (7)	0.8300 (4)	0.0663 (8)	
C13	0.22405 (11)	−0.0462 (9)	1.3047 (5)	0.0626 (10)	
H13	0.2492	−0.1487	1.3296	0.075*	
C12	0.19526 (12)	−0.0669 (10)	1.4255 (5)	0.0623 (10)	
H12	0.2009	−0.1861	1.5283	0.075*	
C11	0.15807 (11)	0.0869 (8)	1.3963 (5)	0.0538 (9)	
H11	0.1389	0.0775	1.4796	0.065*	
C14	0.21666 (10)	0.1221 (8)	1.1479 (5)	0.0550 (9)	
H14	0.2362	0.1344	1.0663	0.066*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

C1	0.045 (2)	0.043 (2)	0.049 (2)	0.000	0.0044 (19)	0.000
O1	0.0553 (12)	0.0652 (16)	0.0487 (12)	0.0067 (13)	0.0246 (10)	−0.0001 (12)
N1	0.0334 (12)	0.0523 (16)	0.0379 (12)	−0.0001 (12)	0.0081 (9)	−0.0005 (12)
C2	0.0318 (13)	0.0395 (16)	0.0429 (15)	−0.0057 (13)	0.0075 (11)	−0.0021 (13)
C6	0.0377 (15)	0.051 (2)	0.0422 (16)	0.0029 (15)	0.0117 (12)	−0.0059 (15)
C7	0.0334 (14)	0.0439 (16)	0.0377 (14)	−0.0041 (13)	0.0080 (11)	0.0002 (14)
C5	0.0512 (17)	0.049 (2)	0.0368 (15)	0.0000 (16)	0.0102 (12)	−0.0059 (14)
C8	0.0449 (16)	0.0454 (18)	0.0343 (14)	−0.0037 (15)	0.0111 (11)	−0.0040 (13)
C3	0.0482 (17)	0.0474 (19)	0.0450 (16)	0.0025 (15)	0.0136 (13)	−0.0088 (15)
C4	0.0424 (16)	0.0526 (19)	0.0354 (14)	0.0019 (14)	0.0085 (12)	−0.0031 (14)
C10	0.0378 (15)	0.0486 (18)	0.0425 (16)	−0.0036 (14)	0.0028 (12)	−0.0029 (14)
C9	0.0327 (14)	0.060 (2)	0.0476 (17)	−0.0019 (15)	0.0086 (12)	0.0007 (16)
C15	0.0368 (15)	0.050 (2)	0.0469 (17)	−0.0035 (14)	0.0040 (13)	−0.0003 (15)
O2	0.0431 (12)	0.099 (2)	0.0623 (14)	0.0104 (14)	0.0237 (11)	0.0237 (15)
C13	0.0462 (18)	0.065 (2)	0.072 (2)	0.0046 (19)	−0.0004 (17)	0.008 (2)
C12	0.061 (2)	0.061 (2)	0.058 (2)	−0.001 (2)	−0.0065 (17)	0.0114 (19)
C11	0.0558 (19)	0.062 (2)	0.0417 (17)	−0.0080 (17)	0.0043 (14)	0.0063 (17)
C14	0.0412 (17)	0.065 (2)	0.058 (2)	0.0027 (16)	0.0072 (15)	0.0041 (18)

Geometric parameters (Å, °)

C1—C2	1.520 (4)	C8—C10	1.479 (4)
C1—C2^{i}	1.520 (4)	C3—H3	0.9300
C1—H1A	0.9700	C4—H4	0.9300
C1—H1B	0.9700	C10—C11	1.376 (5)
O1—C8	1.207 (3)	C10—C15	1.382 (5)
N1—C8	1.412 (4)	C9—O2	1.202 (4)
N1—C9	1.415 (4)	C9—C15	1.484 (5)
N1—C7	1.432 (4)	C15—C14	1.376 (5)
C2—C3	1.376 (4)	C13—C12	1.375 (6)
C2—C4	1.384 (4)	C13—C14	1.377 (5)
C6—C4	1.379 (4)	C13—H13	0.9300
C6—C7	1.385 (4)	C12—C11	1.381 (5)
C6—H6	0.9300	C12—H12	0.9300
C7—C5	1.379 (4)	C11—H11	0.9300
C5—C3	1.386 (4)	C14—H14	0.9300
C5—H5	0.9300		
C2—C1—C2^{i}	112.3 (4)	C5—C3—H3	119.3
C2—C1—H1A	109.1	C6—C4—C2	121.9 (3)
C2^{i}—C1—H1A	109.1	C6—C4—H4	119.1
C2—C1—H1B	109.1	C2—C4—H4	119.1
C2^{i}—C1—H1B	109.1	C11—C10—C15	121.2 (3)
H1A—C1—H1B	107.9	C11—C10—C8	130.3 (3)
C8—N1—C9	110.4 (3)	C15—C10—C8	108.5 (3)
C8—N1—C7	124.6 (2)	O2—C9—N1	125.0 (3)
C9—N1—C7	124.9 (3)	O2—C9—C15	128.9 (3)
C3—C2—C4	117.9 (3)	N1—C9—C15	106.2 (3)
C3—C2—C1	121.3 (3)	C14—C15—C10	121.3 (3)

C4—C2—C1	120.8 (3)	C14—C15—C9	130.2 (3)
C4—C6—C7	119.4 (3)	C10—C15—C9	108.5 (3)
C4—C6—H6	120.3	C12—C13—C14	121.8 (4)
C7—C6—H6	120.3	C12—C13—H13	119.1
C5—C7—C6	119.7 (3)	C14—C13—H13	119.1
C5—C7—N1	120.2 (3)	C13—C12—C11	120.9 (4)
C6—C7—N1	120.0 (3)	C13—C12—H12	119.6
C7—C5—C3	119.9 (3)	C11—C12—H12	119.6
C7—C5—H5	120.1	C10—C11—C12	117.6 (3)
C3—C5—H5	120.1	C10—C11—H11	121.2
O1—C8—N1	125.1 (3)	C12—C11—H11	121.2
O1—C8—C10	128.4 (3)	C15—C14—C13	117.2 (4)
N1—C8—C10	106.5 (3)	C15—C14—H14	121.4
C2—C3—C5	121.3 (3)	C13—C14—H14	121.4
C2—C3—H3	119.3		
C2^{i}—C1—C2—C3	−122.7 (3)	O1—C8—C10—C15	177.8 (3)
C2^{i}—C1—C2—C4	56.4 (2)	N1—C8—C10—C15	−0.7 (3)
C4—C6—C7—C5	0.3 (5)	C8—N1—C9—O2	−178.4 (4)
C4—C6—C7—N1	178.3 (3)	C7—N1—C9—O2	5.5 (5)
C8—N1—C7—C5	40.3 (4)	C8—N1—C9—C15	0.9 (4)
C9—N1—C7—C5	−144.2 (3)	C7—N1—C9—C15	−175.2 (3)
C8—N1—C7—C6	−137.7 (3)	C11—C10—C15—C14	−0.4 (5)
C9—N1—C7—C6	37.8 (4)	C8—C10—C15—C14	−178.1 (3)
C6—C7—C5—C3	−0.3 (5)	C11—C10—C15—C9	179.0 (3)
N1—C7—C5—C3	−178.3 (3)	C8—C10—C15—C9	1.2 (4)
C9—N1—C8—O1	−178.7 (3)	O2—C9—C15—C14	−2.8 (7)
C7—N1—C8—O1	−2.7 (5)	N1—C9—C15—C14	177.9 (3)
C9—N1—C8—C10	−0.1 (3)	O2—C9—C15—C10	178.0 (4)
C7—N1—C8—C10	175.9 (3)	N1—C9—C15—C10	−1.3 (4)
C4—C2—C3—C5	−0.3 (5)	C14—C13—C12—C11	−1.6 (6)
C1—C2—C3—C5	178.8 (3)	C15—C10—C11—C12	−0.9 (5)
C7—C5—C3—C2	0.3 (5)	C8—C10—C11—C12	176.3 (4)
C7—C6—C4—C2	−0.3 (5)	C13—C12—C11—C10	1.8 (6)
C3—C2—C4—C6	0.3 (5)	C10—C15—C14—C13	0.6 (5)
C1—C2—C4—C6	−178.8 (3)	C9—C15—C14—C13	−178.5 (3)
O1—C8—C10—C11	0.4 (6)	C12—C13—C14—C15	0.4 (6)
N1—C8—C10—C11	−178.1 (3)		

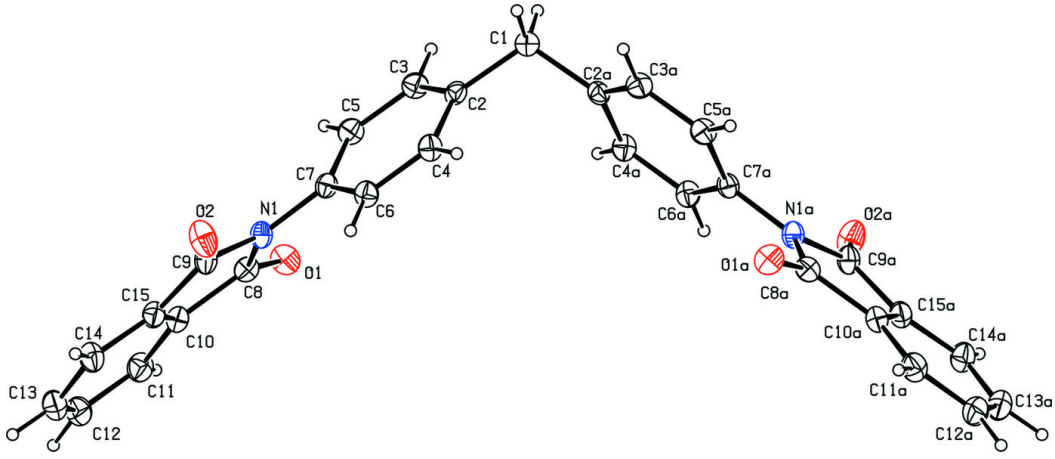
Symmetry codes: (i) −*x*, *y*, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1^{ii}	0.93	2.57	3.251 (4)	131

Symmetry codes: (ii) *x*, *y*, *z*−1.

Fig. 1


C1
C3
C2
C5
C4
C7
C6
O2
N1
C9
O1
C8
C15
C14
C10
C13
C11
C12
C2a
C3a
C5a
C4a
C7a
C6a
N1a
O2a
O1a
C9a
C8a
C15a
C10a
C14a
C11a
C13a
C12a