Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

(Naphthalene-1,4-diyl)dimethyl dibenzoate

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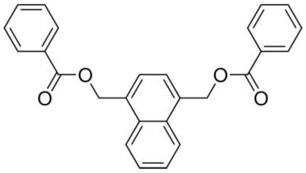
Received 11 January 2010; accepted 4 March 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.081; data-to-parameter ratio = 6.9.

In the title compound, $C_{26}H_{20}O_4$, the complete molecule is generated by a crystallographic 2-fold axis and the naphthalene ring system is planar within 0.05 (4) Å. The dihedral angles between the –COO plane, the benzene ring and naphthalene ring system are 12.83 (3) and 12.93 (1)°, respectively. The –COO plane and the benzene ring are almost coplanar, forming a dihedral angle of 2.59 (8)°.

Related literature

For applications of related naphthalene derivatives, see: Fukuzumi *et al.* (1994); Madsen *et al.* (2002); Strey & Voss (1998); Tsukada *et al.* (1994).



Experimental

Crystal data

$C_{26}H_{20}O_4$	M_r = 396.42
Orthorhombic, $Fdd2$	Z = 8
a = 3.9919 (6) Å	Mo $K\alpha$ radiation
b = 60.385 (8) Å	μ = 0.09 mm^{-1}
c = 16.231 (2) Å	T = 296 K
V = 3912.5 (9) Å^3	0.50 × 0.38 × 0.07 mm

Data collection

Bruker APEXII diffractometer	6343 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	937 independent reflections
T_{min} = 0.957, T_{max} = 0.994	822 reflections with $I > 2\sigma(I)$
	R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033	1 restraint
$wR(F^2)$ = 0.081	H-atom parameters constrained
S = 1.08	$\Delta\rho_{max}$ = 0.10 e Å^{-3}
937 reflections	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
136 parameters	

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Science and Technology Foundation of Zunyi City of China (No. 200723)

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2316).

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supplementary materials

Acta Cryst. (2010). E**66**, o860 [**doi:10.1107/S1600536810008391**]

(Naphthalene-1,4-diyl)dimethyl dibenzoate

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Comment

Numerous 1,4-naphthalene derivatives have been synthesized and studied. 1,4-naphthalene derivatives are important intermediates for applications such as monomers in the preparation of polymers (Fukuzumi *et al.*, 1994; Tsukada *et al.*, 1994). The title compound has a 2-fold axis of symmetry passing through the long axis of napthalene (Fig. 1). The naphthalene ring system is planar within 0.05 (4)A°. The dihedral angles of the C1/O1/O2 plane, the C2—C7 ring and naphthalene ring are 12.83 (3)° and 12.93 (1)°, respectively. Molecules of the title compound are closely stacked with a repeat equal to the a-axial dimension.

Experimental

The title compound was synthesized according to the reported procedure of Strey & Voss (1998) and Madsen *et al.* (2002). Colourless single crystals suitable for X-ray diffraction were obtained by recrystallization from ethyl acetate.

Refinement

H atoms were positioned geometrically, with C-H = 0.93 and 0.97Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, Uiso(H)= 1.2Ueq(C). In the absence of significant anomalous scattering, Friedel opposites were merged (862 Friedel pairs).

Figures

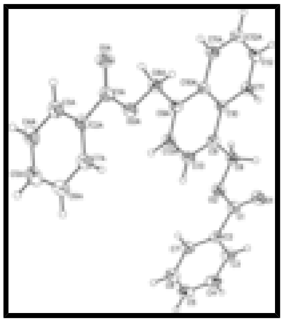

Fig. 1. The molecular structure of the title compound showing 30% probability displacement ellipsoids and the atomic numbering. Symmetry code: A = 1.5 -x,0.5-y, z.

(Naphthalene-1,4-diyl)dimethyl dibenzoate

Crystal data

$C_{26}H_{20}O_4$	$F(000) = 1664$
$M_r = 396.42$	$D_x = 1.346$ Mg m^{-3}
Orthorhombic, *Fdd*2	Mo *Kα* radiation, λ = 0.71073 Å

Hall symbol: F 2 -2 d

a = 3.9919 (6) Å

b = 60.385 (8) Å

c = 16.231 (2) Å

V = 3912.5 (9) $Å^3$

Z = 8

Cell parameters from 1789 reflections

θ = 2.6–25.3°

μ = 0.09 mm^{-1}

T = 296 K

Block, colourless

0.50 × 0.38 × 0.07 mm

Data collection

Bruker APEXII diffractometer

Radiation source: fine-focus sealed tube

graphite

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.957, T_{max} = 0.994

6343 measured reflections

937 independent reflections

822 reflections with $I > 2\sigma(I)$

R_{int} = 0.027

θ_{max} = 25.5°, θ_{min} = 2.6°

$h = -4 \rightarrow 4$

$k = -72 \rightarrow 72$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.033

$wR(F^2)$ = 0.081

S = 1.08

937 reflections

136 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ < 0.001

$\Delta\rho_{max}$ = 0.10 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.15 e $Å^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 > 2sigma(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}

O1	0.1416 (5)	0.16848 (3)	0.65497 (12)	0.0680 (6)
O2	0.4250 (4)	0.19760 (2)	0.60506 (10)	0.0507 (4)
C1	0.2722 (6)	0.17767 (3)	0.59764 (15)	0.0467 (5)
C2	0.2903 (6)	0.16879 (3)	0.51236 (15)	0.0452 (5)
C3	0.1552 (6)	0.14804 (3)	0.49816 (16)	0.0556 (7)
H3	0.0516	0.1404	0.5408	0.067*
C4	0.1746 (8)	0.13876 (4)	0.42042 (17)	0.0652 (8)
H4	0.0881	0.1247	0.4112	0.078*
C5	0.3209 (7)	0.15021 (4)	0.35675 (18)	0.0655 (7)
H5	0.3302	0.1440	0.3044	0.079*
C6	0.4533 (7)	0.17084 (4)	0.37037 (17)	0.0611 (7)
H6	0.5522	0.1786	0.3272	0.073*
C7	0.4407 (7)	0.18018 (4)	0.44775 (16)	0.0522 (6)
H7	0.5328	0.1941	0.4568	0.063*
C8	0.4461 (6)	0.20608 (3)	0.68748 (14)	0.0455 (5)
H8A	0.5784	0.1961	0.7213	0.055*
H8B	0.2236	0.2071	0.7112	0.055*
C9	0.6053 (5)	0.22851 (3)	0.68603 (13)	0.0413 (5)
C10	0.6767 (5)	0.23923 (3)	0.76281 (14)	0.0391 (5)
C11	0.6072 (6)	0.22913 (4)	0.83964 (14)	0.0474 (6)
H11	0.5109	0.2151	0.8405	0.057*
C12	0.6774 (7)	0.23935 (4)	0.91223 (14)	0.0537 (6)
H12	0.6296	0.2323	0.9618	0.064*
C13	0.6778 (6)	0.23930 (4)	0.61428 (14)	0.0468 (6)
H13	0.6314	0.2324	0.5643	0.056*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0943 (15)	0.0554 (11)	0.0542 (11)	−0.0234 (10)	0.0100 (11)	0.0017 (9)
O2	0.0665 (11)	0.0417 (8)	0.0440 (9)	−0.0096 (7)	0.0002 (8)	−0.0032 (7)
C1	0.0565 (14)	0.0351 (10)	0.0486 (13)	−0.0024 (10)	−0.0037 (11)	0.0034 (11)
C2	0.0506 (13)	0.0390 (11)	0.0458 (13)	0.0011 (9)	−0.0074 (10)	0.0022 (10)
C3	0.0679 (17)	0.0407 (12)	0.0582 (17)	−0.0059 (11)	−0.0134 (13)	0.0024 (11)
C4	0.087 (2)	0.0445 (13)	0.0640 (18)	−0.0039 (13)	−0.0223 (15)	−0.0045 (13)
C5	0.084 (2)	0.0592 (15)	0.0538 (15)	0.0109 (14)	−0.0130 (14)	−0.0110 (14)
C6	0.0730 (18)	0.0615 (16)	0.0488 (15)	0.0047 (13)	0.0000 (13)	0.0010 (12)
C7	0.0627 (15)	0.0423 (11)	0.0517 (14)	−0.0017 (11)	−0.0027 (12)	0.0001 (11)
C8	0.0526 (13)	0.0420 (11)	0.0418 (13)	−0.0017 (10)	−0.0006 (11)	−0.0024 (11)
C9	0.0441 (13)	0.0398 (11)	0.0399 (13)	0.0027 (9)	−0.0010 (10)	0.0006 (10)
C10	0.0412 (11)	0.0398 (10)	0.0362 (11)	0.0054 (9)	0.0006 (10)	0.0003 (10)
C11	0.0558 (15)	0.0422 (11)	0.0442 (13)	−0.0007 (10)	0.0014 (12)	0.0053 (11)
C12	0.0667 (17)	0.0573 (14)	0.0371 (13)	0.0034 (11)	0.0039 (12)	0.0064 (10)
C13	0.0598 (14)	0.0445 (11)	0.0362 (12)	−0.0047 (10)	−0.0032 (11)	−0.0040 (10)

Geometric parameters (Å, °)

O1—C1	1.202 (3)	C7—H7	0.9300
O2—C1	1.354 (3)	C8—C9	1.496 (3)

O2—C8	1.435 (3)	C8—H8A	0.9700
C1—C2	1.486 (3)	C8—H8B	0.9700
C2—C3	1.384 (3)	C9—C13	1.365 (3)
C2—C7	1.390 (3)	C9—C10	1.433 (3)
C3—C4	1.383 (4)	C10—C11	1.416 (3)
C3—H3	0.9300	C10—C10^{i}	1.426 (4)
C4—C5	1.374 (4)	C11—C12	1.359 (3)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.371 (4)	C12—C12^{i}	1.410 (5)
C5—H5	0.9300	C12—H12	0.9300
C6—C7	1.378 (4)	C13—C13^{i}	1.415 (4)
C6—H6	0.9300	C13—H13	0.9300

C1—O2—C8	115.25 (18)	O2—C8—C9	109.48 (18)
O1—C1—O2	122.4 (2)	O2—C8—H8A	109.8
O1—C1—C2	125.1 (2)	C9—C8—H8A	109.8
O2—C1—C2	112.43 (19)	O2—C8—H8B	109.8
C3—C2—C7	119.4 (2)	C9—C8—H8B	109.8
C3—C2—C1	117.6 (2)	H8A—C8—H8B	108.2
C7—C2—C1	123.03 (19)	C13—C9—C10	118.96 (18)
C4—C3—C2	119.8 (2)	C13—C9—C8	122.36 (19)
C4—C3—H3	120.1	C10—C9—C8	118.67 (18)
C2—C3—H3	120.1	C11—C10—C10^{i}	118.26 (12)
C5—C4—C3	120.4 (2)	C11—C10—C9	122.17 (17)
C5—C4—H4	119.8	C10^{i}—C10—C9	119.57 (11)
C3—C4—H4	119.8	C12—C11—C10	121.8 (2)
C6—C5—C4	120.0 (3)	C12—C11—H11	119.1
C6—C5—H5	120.0	C10—C11—H11	119.1
C4—C5—H5	120.0	C11—C12—C12^{i}	119.92 (13)
C5—C6—C7	120.3 (3)	C11—C12—H12	120.0
C5—C6—H6	119.8	C12^{i}—C12—H12	120.0
C7—C6—H6	119.8	C9—C13—C13^{i}	121.47 (12)
C6—C7—C2	120.1 (2)	C9—C13—H13	119.3
C6—C7—H7	120.0	C13^{i}—C13—H13	119.3
C2—C7—H7	120.0		

C8—O2—C1—O1	5.3 (3)	C1—C2—C7—C6	179.0 (2)
C8—O2—C1—C2	−174.01 (19)	C1—O2—C8—C9	−177.40 (18)
O1—C1—C2—C3	−2.0 (4)	O2—C8—C9—C13	6.7 (3)
O2—C1—C2—C3	177.2 (2)	O2—C8—C9—C10	−174.77 (18)
O1—C1—C2—C7	179.2 (3)	C13—C9—C10—C11	179.7 (2)
O2—C1—C2—C7	−1.6 (3)	C8—C9—C10—C11	1.2 (3)
C7—C2—C3—C4	0.8 (4)	C13—C9—C10—C10^{i}	−0.4 (3)
C1—C2—C3—C4	−178.1 (2)	C8—C9—C10—C10^{i}	−179.0 (2)
C2—C3—C4—C5	−1.4 (4)	C10^{i}—C10—C11—C12	−0.2 (4)
C3—C4—C5—C6	1.0 (4)	C9—C10—C11—C12	179.7 (2)
C4—C5—C6—C7	0.0 (4)	C10—C11—C12—C12^{i}	0.2 (5)
C5—C6—C7—C2	−0.6 (4)	C10—C9—C13—C13^{i}	0.2 (4)

C3—C2—C7—C6	0.2 (4)	C8—C9—C13—C13^{i}	178.7 (3)

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

Fig. 1