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2-(2,3-Dimethylphenyl)-1*H*-isoindole-1,3(2*H*)-dione

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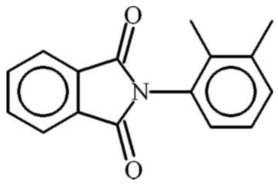
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.097; data-to-parameter ratio = 13.4.

In the title compound, $C_{16}H_{13}NO_2$, the 2,3-dimethylphenyl group and the 1*H*-isoindole-1,3(2*H*)-dione group are essentially planar, with r.m.s. deviations of 0.006 and 0.013 Å, respectively, and are oriented at an angle of 78.19 (3)° with respect to each other. In the crystal, weak C—H⋯O interactions link the molecules, forming a zigzag chain parallel to the b axis. Futhermore, C—H⋯π interactions are present between the C—H group of isoindole and the 2,3-dimethylphenyl benzene ring. The H atoms of the *ortho*-methyl group are statistically disordered over two positions. Such disorder might be related to the antagonism between intramolecular steric repulsions and intermolecular C—H⋯O interactions.

Related literature

For background to Schiff bases containing 2,3-dimethylaniline and for related structures, see: Bocelli & Cantoni (1989); Chandrashekar *et al.* (1983); Izotova *et al.* (2009); Sarfraz *et al.* (2010); Tahir *et al.* (2010); Tariq *et al.* (2010).



Experimental

Crystal data

$C_{16}H_{13}NO_2$
M_r = 251.27
Monoclinic, $P2_1/c$
a = 7.8222 (3) Å
b = 8.4576 (3) Å
c = 19.4863 (6) Å
β = 91.441 (2)°
V = 1288.75 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.30 × 0.12 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min}$ = 0.980, $T_{\max}$ = 0.993
9849 measured reflections
2320 independent reflections
1819 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.097
S = 1.04
2320 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.13 e Å^{-3}
$\Delta\rho_{\min}$ = −0.13 e Å^{-3}

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

*Cg*2 is the centroid of the C1—C6 ring.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C7—H7F⋯O1$^{\rm i}$	0.96	2.52	3.3486 (19)	145
C8—H8C⋯$Cg2^{\rm ii}$	0.96	2.89	3.5644 (18)	128
C11—H11⋯$Cg2^{\rm iii}$	0.93	2.77	3.6798 (15)	166

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2596).

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supplementary materials

Acta Cryst. (2010). E**66**, o2440   [**doi:10.1107/S1600536810033386**]

2-(2,3-Dimethylphenyl)-1*H*-isoindole-1,3(2*H*)-dione

M. I. Tariq, T. Noreen, M. N. Tahir, S. Ahmad and M. Fayyaz-ur-Rehman

Comment

We have reported crystal structures of Schiff bases containing 2,3-dimethylaniline (Sarfraz *et al.*, 2010), (Tahir *et al.*, 2010) and (Tariq *et al.*, 2010). As part of our continuing interest in Schiff bases containing 2,3-dimethylaniline, we report here the structure of the title compound (I).

The crystal structure of related compounds (II), *N*-phenylphthalimide (Izotova *et al.*, 2009), (III) *N*-*m*-tolylphthalimide (Chandrashekar *et al.*, 1983) and (IV) *N*-(*o*-tolyl)phthalimide (Bocelli & Cantoni, 1989) have been already published.

In (I), the 2,3-dimethylanilinic moiety A (C1—C8) and the 1*H*-isoindole-1,3(2*H*)-dione group B (C9—C15/N1/O1/O2) are planar with r. m. s. deviations of 0.0056 and 0.0131 Å, respectively. The dihedral angle between A/B is 78.19 (3)° (Fig. 1).

The H-atoms of the *ortho*-methyl group are statistically disordered over two positions. Such disorder might be related to the antagonism between intramolecular C-H···N and intermolecular C-H···O interactions (Table 1). The weak C—H···O interactions links the molecule forming a non continuous zig-zag chain parallel to the b axis owing to the statistical distribution of the H atoms. Weak C-H···π interactions are also present (Table 1, where Cg2 is the centroid of the phenyl ring C1—C6).

Experimental

Equimolar quantities of 2,3-dimethylaniline and phthalic anhydride were refluxed in methanol for 48 h. The solution was kept at room temperature which affoarded white prism after 48 h.

Refinement

The H-atoms were positioned geometrically (C–H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl and x = 1.2 for aryl H-atoms.

The difference Fourier map showed that H-atoms of *ortho*-methyl are disordered. They were then geometrically located and treated as riding using the tools (AFIX 123) available in SHELXL97 (Sheldrick, 2008)

Figures

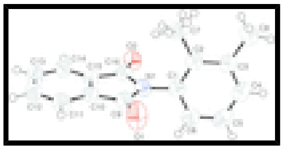

Fig. 1. View of the title compound with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level. H-atoms are represented by small circles of arbitrary radii.

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Crystal data

$C_{16}H_{13}NO_2$
$M_r = 251.27$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.8222$ (3) Å
$b = 8.4576$ (3) Å
$c = 19.4863$ (6) Å
$\beta = 91.441$ (2)°
$V = 1288.75$ (8) Å^3
$Z = 4$

$F(000) = 528$
$D_x = 1.295$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1819 reflections
$\theta = 2.6$–25.2°
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Prism, white
0.30 × 0.12 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
graphite
Detector resolution: 8.10 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min} = 0.980$, $T_{\max} = 0.993$
9849 measured reflections

2320 independent reflections
1819 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.029$
$\theta_{\max} = 25.2°$, $\theta_{\min} = 2.6°$
$h = -8 \rightarrow 9$
$k = -10 \rightarrow 10$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.097$
$S = 1.04$
2320 reflections
173 parameters
0 restraints

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
$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.2276P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.13$ 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 $F^2 > \sigma(F^2)$ 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	$U_{\rm iso}$*/$U_{\rm eq}$	Occ. (<1)
O1	0.49485 (18)	0.42949 (17)	0.22907 (6)	0.0925 (5)	
O2	0.79930 (14)	0.38827 (14)	0.03357 (5)	0.0628 (3)	
N1	0.61379 (16)	0.38436 (14)	0.12397 (6)	0.0490 (3)	
C1	0.49387 (19)	0.26593 (18)	0.10015 (7)	0.0467 (4)	
C2	0.53838 (18)	0.10792 (18)	0.10503 (6)	0.0450 (4)	
C3	0.41581 (19)	−0.00524 (18)	0.08357 (7)	0.0489 (4)	
C4	0.2583 (2)	0.0467 (2)	0.05916 (7)	0.0598 (4)	
H4	0.1775	−0.0278	0.0449	0.072*	
C5	0.2167 (2)	0.2044 (2)	0.05521 (8)	0.0671 (5)	
H5	0.1092	0.2354	0.0388	0.080*	
C6	0.3357 (2)	0.3165 (2)	0.07580 (8)	0.0579 (4)	
H6	0.3099	0.4237	0.0733	0.069*	
C7	0.7094 (2)	0.0574 (2)	0.13251 (8)	0.0591 (4)	
H7A	0.7165	−0.0559	0.1318	0.089*	0.50
H7B	0.7247	0.0945	0.1788	0.089*	0.50
H7C	0.7970	0.1010	0.1046	0.089*	0.50
H7D	0.7756	0.1490	0.1450	0.089*	0.50
H7E	0.7675	−0.0015	0.0980	0.089*	0.50
H7F	0.6951	−0.0079	0.1723	0.089*	0.50
C8	0.4548 (2)	−0.1781 (2)	0.08813 (9)	0.0665 (5)	
H8A	0.3620	−0.2372	0.0677	0.100*	
H8B	0.4697	−0.2079	0.1354	0.100*	
H8C	0.5579	−0.2001	0.0642	0.100*	
C9	0.6040 (2)	0.45618 (19)	0.18862 (7)	0.0555 (4)	
C10	0.75207 (18)	0.56363 (17)	0.19457 (7)	0.0457 (4)	
C11	0.8017 (2)	0.66315 (19)	0.24722 (7)	0.0562 (4)	
H11	0.7393	0.6707	0.2871	0.067*	
C12	0.9479 (2)	0.7513 (2)	0.23830 (8)	0.0622 (4)	
H12	0.9848	0.8199	0.2729	0.075*	
C13	1.0403 (2)	0.7399 (2)	0.17923 (9)	0.0652 (5)	
H13	1.1387	0.8005	0.1749	0.078*	
C14	0.9898 (2)	0.6399 (2)	0.12609 (8)	0.0565 (4)	
H14	1.0520	0.6326	0.0862	0.068*	
C15	0.84406 (18)	0.55212 (16)	0.13486 (7)	0.0432 (3)	
C16	0.75805 (19)	0.43515 (17)	0.08932 (7)	0.0463 (4)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0969 (10)	0.1151 (11)	0.0678 (8)	−0.0452 (9)	0.0465 (8)	−0.0311 (7)
O2	0.0700 (8)	0.0772 (8)	0.0420 (6)	−0.0077 (6)	0.0174 (5)	−0.0097 (5)
N1	0.0550 (8)	0.0515 (7)	0.0412 (6)	−0.0075 (6)	0.0130 (5)	−0.0041 (5)
C1	0.0521 (9)	0.0521 (9)	0.0363 (7)	−0.0015 (7)	0.0086 (6)	−0.0002 (6)
C2	0.0462 (8)	0.0558 (9)	0.0332 (7)	0.0017 (7)	0.0064 (6)	0.0019 (6)
C3	0.0528 (9)	0.0580 (9)	0.0364 (7)	−0.0068 (7)	0.0081 (6)	0.0004 (6)
C4	0.0569 (10)	0.0754 (12)	0.0469 (9)	−0.0121 (9)	0.0012 (7)	0.0016 (8)
C5	0.0491 (10)	0.0938 (14)	0.0580 (10)	0.0064 (10)	−0.0028 (8)	0.0117 (9)
C6	0.0560 (10)	0.0646 (10)	0.0532 (9)	0.0073 (8)	0.0041 (7)	0.0079 (8)
C7	0.0575 (10)	0.0606 (10)	0.0591 (9)	0.0025 (8)	0.0014 (8)	0.0047 (8)
C8	0.0784 (13)	0.0584 (10)	0.0630 (10)	−0.0083 (9)	0.0117 (9)	−0.0041 (8)
C9	0.0642 (10)	0.0581 (10)	0.0450 (8)	−0.0058 (8)	0.0175 (7)	−0.0056 (7)
C10	0.0514 (9)	0.0451 (8)	0.0410 (7)	0.0039 (7)	0.0063 (6)	0.0009 (6)
C11	0.0627 (11)	0.0614 (10)	0.0450 (8)	0.0008 (8)	0.0077 (7)	−0.0068 (7)
C12	0.0637 (11)	0.0645 (11)	0.0581 (10)	−0.0053 (9)	−0.0037 (8)	−0.0118 (8)
C13	0.0554 (10)	0.0726 (12)	0.0677 (11)	−0.0122 (9)	0.0030 (8)	−0.0031 (9)
C14	0.0520 (10)	0.0662 (10)	0.0516 (9)	−0.0021 (8)	0.0103 (7)	0.0020 (8)
C15	0.0460 (8)	0.0444 (8)	0.0394 (7)	0.0049 (7)	0.0045 (6)	0.0039 (6)
C16	0.0507 (9)	0.0494 (9)	0.0392 (7)	0.0038 (7)	0.0090 (6)	0.0029 (6)

Geometric parameters (Å, °)

O1—C9	1.1982 (17)	C7—H7D	0.9600
O2—C16	1.2079 (16)	C7—H7E	0.9600
N1—C16	1.3972 (17)	C7—H7F	0.9600
N1—C9	1.4025 (18)	C8—H8A	0.9600
N1—C1	1.4411 (19)	C8—H8B	0.9600
C1—C6	1.382 (2)	C8—H8C	0.9600
C1—C2	1.384 (2)	C9—C10	1.474 (2)
C2—C3	1.411 (2)	C10—C11	1.375 (2)
C2—C7	1.491 (2)	C10—C15	1.3867 (18)
C3—C4	1.381 (2)	C11—C12	1.380 (2)
C3—C8	1.496 (2)	C11—H11	0.9300
C4—C5	1.375 (3)	C12—C13	1.378 (2)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.381 (2)	C13—C14	1.386 (2)
C5—H5	0.9300	C13—H13	0.9300
C6—H6	0.9300	C14—C15	1.375 (2)
C7—H7A	0.9600	C14—H14	0.9300
C7—H7B	0.9600	C15—C16	1.479 (2)
C7—H7C	0.9600		

C16—N1—C9	111.33 (12)	C2—C7—H7F	109.5
C16—N1—C1	125.81 (11)	H7A—C7—H7F	56.3
C9—N1—C1	122.73 (11)	H7B—C7—H7F	56.3

C6—C1—C2	122.96 (14)	H7C—C7—H7F	141.1
C6—C1—N1	117.74 (14)	H7D—C7—H7F	109.5
C2—C1—N1	119.25 (13)	H7E—C7—H7F	109.5
C1—C2—C3	117.84 (14)	C3—C8—H8A	109.5
C1—C2—C7	121.57 (14)	C3—C8—H8B	109.5
C3—C2—C7	120.59 (14)	H8A—C8—H8B	109.5
C4—C3—C2	118.69 (15)	C3—C8—H8C	109.5
C4—C3—C8	120.68 (15)	H8A—C8—H8C	109.5
C2—C3—C8	120.62 (15)	H8B—C8—H8C	109.5
C5—C4—C3	122.39 (16)	O1—C9—N1	124.41 (15)
C5—C4—H4	118.8	O1—C9—C10	129.49 (14)
C3—C4—H4	118.8	N1—C9—C10	106.09 (11)
C4—C5—C6	119.53 (16)	C11—C10—C15	121.76 (14)
C4—C5—H5	120.2	C11—C10—C9	129.95 (13)
C6—C5—H5	120.2	C15—C10—C9	108.29 (12)
C5—C6—C1	118.59 (16)	C10—C11—C12	117.11 (14)
C5—C6—H6	120.7	C10—C11—H11	121.4
C1—C6—H6	120.7	C12—C11—H11	121.4
C2—C7—H7A	109.5	C13—C12—C11	121.42 (15)
C2—C7—H7B	109.5	C13—C12—H12	119.3
H7A—C7—H7B	109.5	C11—C12—H12	119.3
C2—C7—H7C	109.5	C12—C13—C14	121.41 (16)
H7A—C7—H7C	109.5	C12—C13—H13	119.3
H7B—C7—H7C	109.5	C14—C13—H13	119.3
C2—C7—H7D	109.5	C15—C14—C13	117.26 (14)
H7A—C7—H7D	141.1	C15—C14—H14	121.4
H7B—C7—H7D	56.3	C13—C14—H14	121.4
H7C—C7—H7D	56.3	C14—C15—C10	121.05 (13)
C2—C7—H7E	109.5	C14—C15—C16	130.74 (12)
H7A—C7—H7E	56.3	C10—C15—C16	108.21 (12)
H7B—C7—H7E	141.1	O2—C16—N1	124.82 (14)
H7C—C7—H7E	56.3	O2—C16—C15	129.14 (13)
H7D—C7—H7E	109.5	N1—C16—C15	106.04 (11)

Hydrogen-bond geometry (Å, °)

Cg2 is the centroid of the C1—C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7D···N1	0.96	2.39	2.868 (2)	110.
C7—H7F···O1^{i}	0.96	2.52	3.3486 (19)	145.
C8—H8C···Cg2^{ii}	0.96	2.89	3.5644 (18)	128
C11—H11···Cg2^{iii}	0.93	2.77	3.6798 (15)	166

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

Fig. 1