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

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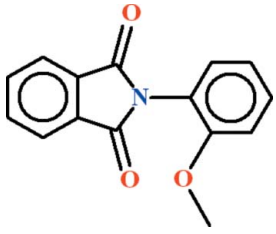
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.112; data-to-parameter ratio = 14.0.

In the title compound, $C_{15}H_{11}NO_3$, the dihedral angle between the methoxybenzene and isoindole ring systems is 70.21 (3)°. The methoxy C atom is close to being coplanar with its attached ring [deviation = 0.133 (2) Å] and is oriented away from the isoindole moiety. In the crystal, inversion dimers linked by pairs of C—H···O hydrogen bonds generate $R_2^2(10)$ loops. Further C—H···O interactions lead to (010) infinite sheets and weak aromatic π–π stacking [centroid–centroid separations = 3.6990 (10) and 3.7217 (10) Å] is also observed.

Related literature

For related structures, see: Sim *et al.* (2009); Sirajuddin *et al.* (2012). For hydrogen-bond motifs, see: Bernstein *et al.*, 1995).



Experimental

Crystal data

$C_{15}H_{11}NO_3$
M_r = 253.25
Orthorhombic, *Pbca*
a = 11.5768 (6) Å
b = 7.3222 (5) Å
c = 29.2849 (15) Å
V = 2482.4 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.32 × 0.26 × 0.24 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.969, T_{max} = 0.977
10815 measured reflections
2428 independent reflections
1816 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
S = 1.03
2428 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1^{i}	0.93	2.57	3.428 (2)	153
C12—H12···O2^{ii}	0.93	2.46	3.313 (2)	152

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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 a 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: HB6857).

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supporting information

Acta Cryst. (2012). E**68**, o2589 [https://doi.org/10.1107/S1600536812027262]

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

M. Nawaz Tahir, Muhammad Sirajuddin, Saqib Ali and Khurram Shahzad Munawar

S1. Comment

The title compound (I), (Fig. 1) has been synthesized in an attempt to form the carboxylic acid containing methoxybenzene. We have reported the crystal structure of 1-(2-methoxyphenyl)-1*H*-pyrrole-2,5-dione (Sirajuddin *et al.*, 2012) which is related to (I). The polymorph of (I) has also been published by (Sim *et al.*, 2009).

In (I), 1*H*-isoindole-1,3(2*H*)-dione A (C1—C8/N1/O1/O2) and the methoxybenzene B (C9—C15/O3) are almost planar with r.m.s. deviation of 0.0458 and 0.0320 Å, respectively. The dihedral angle between A/B is 70.21 (3)°. The molecules are dimerized due to C—H···O type of H-bonding with $R_2^2(10)$ ring motifs (Bernstein *et al.*, 1995). The dimers are interlinked due to further C—H···O bonds to form infinite sheets. There exist $\pi\cdots\pi$ interaction between *Cg*1···*Cg*2^{i} [i = 3/2 - *x*, -1/2 + *y*, *z*] and *Cg*2···*Cg*1^{ii} [ii = 3/2 - *x*, 1/2 + *y*, *z*] at a distance of 3.7217 (10) Å. Similarly, there exist $\pi\cdots\pi$ interaction between *Cg*2··· *Cg*2^{i} [i = 3/2 - *x*, -1/2 + *y*, *z*] and *Cg*2··· *Cg*2^{ii} [ii = 3/2 - *x*, 1/2 + *y*, *z*] at a distance of 3.6990 (10) Å. *Cg*1 and *Cg*2 are the centroids of (C1/C2/C7/C8/N1) and (C2—C7) rings, respectively.

S2. Experimental

Equimolar quantities of 2-methoxyaniline and phthalic anhydride were stirred and refluxed in acetic acid for 4 h. The solution was kept at room temperature which afforded dark yellow prisms after 12 h.

S3. 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 other H-atoms.

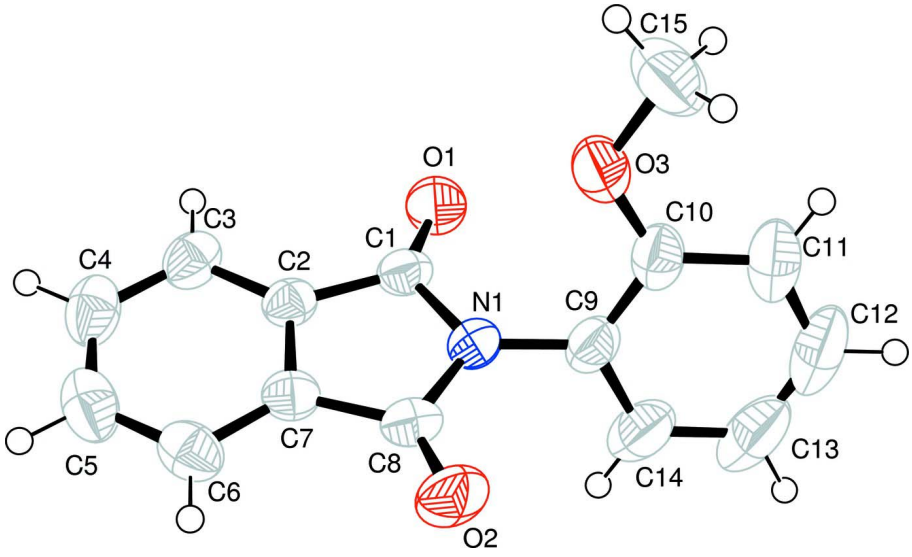

Figure 1

View of the title compound with displacement ellipsoids drawn at the 50% probability level.

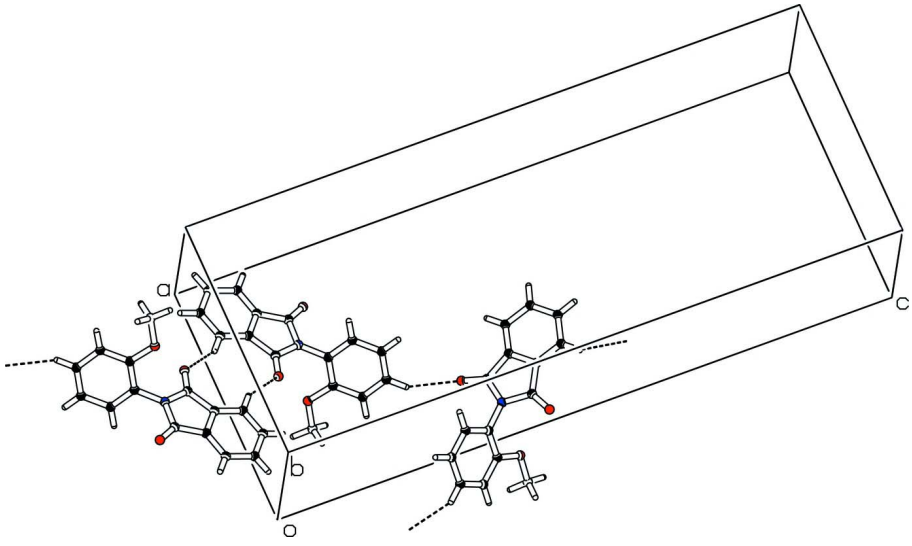

Figure 2

The partial packing, which shows that molecules form dimers with $R_2^2(10)$ ring mtifs and C(18) chains are formed due to C—H···O bonds.

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

Crystal data

$C_{15}H_{11}NO_3$
M_r = 253.25
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 11.5768 (6) Å
b = 7.3222 (5) Å
c = 29.2849 (15) Å
V = 2482.4 (2) Å^3
Z = 8
F(000) = 1056
D_x = 1.355 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1816 reflections
θ = 2.2–26.0°

μ = 0.10 mm^{-1}
T = 296 K

Prism, dark yellow
0.32 × 0.26 × 0.24 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.969, T_{max} = 0.977

10815 measured reflections
2428 independent reflections
1816 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 26.0°, θ_{min} = 2.2°
h = −14→14
k = −9→5
l = −35→36

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
S = 1.03
2428 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
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.6208P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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_{iso}*/U_{eq}
O1	0.45483 (10)	0.37357 (19)	0.07121 (4)	0.0609 (4)
O2	0.74031 (12)	0.1478 (2)	0.16275 (4)	0.0672 (5)
O3	0.41409 (11)	−0.01341 (19)	0.11923 (4)	0.0632 (5)
N1	0.57642 (11)	0.2519 (2)	0.12589 (4)	0.0451 (4)
C1	0.54983 (14)	0.3245 (2)	0.08300 (5)	0.0432 (5)
C2	0.66018 (14)	0.3329 (2)	0.05763 (5)	0.0409 (5)
C3	0.68405 (17)	0.3932 (2)	0.01415 (6)	0.0512 (6)
C4	0.79860 (18)	0.3945 (3)	0.00060 (6)	0.0607 (6)
C5	0.88538 (17)	0.3416 (3)	0.02983 (7)	0.0635 (7)
C6	0.86140 (15)	0.2806 (2)	0.07348 (7)	0.0551 (6)
C7	0.74722 (14)	0.2752 (2)	0.08649 (5)	0.0422 (5)
C8	0.69509 (14)	0.2162 (2)	0.13013 (5)	0.0454 (5)
C9	0.49518 (15)	0.2254 (3)	0.16170 (5)	0.0501 (5)
C10	0.41319 (15)	0.0874 (3)	0.15822 (6)	0.0530 (6)

C11	0.33615 (18)	0.0624 (3)	0.19381 (7)	0.0716 (8)
C12	0.3427 (2)	0.1736 (4)	0.23180 (7)	0.0881 (9)
C13	0.4240 (2)	0.3075 (4)	0.23528 (7)	0.0922 (10)
C14	0.5005 (2)	0.3346 (3)	0.19983 (6)	0.0724 (8)
C15	0.3388 (2)	−0.1661 (3)	0.11653 (9)	0.0873 (10)
H3	0.62552	0.43151	−0.00537	0.0615*
H4	0.81725	0.43190	−0.02884	0.0728*
H5	0.96171	0.34706	0.02003	0.0762*
H6	0.92002	0.24465	0.09325	0.0661*
H11	0.28034	−0.02875	0.19216	0.0860*
H12	0.29047	0.15681	0.25555	0.1058*
H13	0.42784	0.37989	0.26133	0.1107*
H14	0.55562	0.42669	0.20171	0.0869*
H15A	0.35417	−0.24768	0.14146	0.1309*
H15B	0.35107	−0.22876	0.08815	0.1309*
H15C	0.26011	−0.12507	0.11816	0.1309*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0466 (7)	0.0825 (9)	0.0537 (7)	0.0051 (6)	−0.0098 (6)	0.0129 (6)
O2	0.0672 (8)	0.0852 (10)	0.0493 (7)	0.0108 (7)	−0.0175 (6)	0.0115 (7)
O3	0.0594 (8)	0.0663 (8)	0.0640 (8)	−0.0159 (7)	0.0127 (6)	−0.0053 (7)
N1	0.0446 (7)	0.0554 (8)	0.0354 (7)	−0.0026 (6)	−0.0048 (6)	0.0049 (6)
C1	0.0469 (9)	0.0450 (9)	0.0377 (8)	−0.0029 (7)	−0.0084 (7)	0.0011 (7)
C2	0.0486 (9)	0.0354 (8)	0.0386 (8)	−0.0039 (7)	−0.0041 (7)	−0.0020 (7)
C3	0.0687 (11)	0.0425 (9)	0.0424 (9)	−0.0034 (8)	−0.0003 (8)	0.0020 (7)
C4	0.0791 (13)	0.0484 (10)	0.0546 (10)	−0.0081 (10)	0.0193 (10)	0.0008 (9)
C5	0.0580 (11)	0.0530 (11)	0.0794 (14)	−0.0071 (9)	0.0204 (10)	−0.0039 (10)
C6	0.0472 (10)	0.0479 (10)	0.0701 (12)	−0.0016 (8)	−0.0024 (9)	−0.0064 (9)
C7	0.0466 (9)	0.0350 (8)	0.0451 (9)	−0.0031 (7)	−0.0037 (7)	−0.0049 (7)
C8	0.0497 (9)	0.0450 (9)	0.0414 (9)	−0.0003 (7)	−0.0116 (7)	−0.0016 (7)
C9	0.0507 (9)	0.0640 (11)	0.0356 (8)	0.0064 (9)	−0.0014 (7)	0.0044 (8)
C10	0.0499 (10)	0.0628 (11)	0.0464 (9)	0.0077 (9)	0.0064 (8)	0.0125 (9)
C11	0.0632 (12)	0.0882 (16)	0.0635 (12)	0.0137 (11)	0.0195 (10)	0.0266 (12)
C12	0.0832 (16)	0.131 (2)	0.0502 (12)	0.0392 (16)	0.0234 (12)	0.0282 (14)
C13	0.1046 (19)	0.131 (2)	0.0410 (11)	0.0330 (18)	0.0029 (12)	−0.0085 (13)
C14	0.0815 (14)	0.0915 (16)	0.0442 (10)	0.0069 (12)	−0.0051 (10)	−0.0098 (10)
C15	0.0696 (14)	0.0819 (16)	0.1103 (19)	−0.0268 (12)	0.0106 (13)	−0.0047 (14)

Geometric parameters (Å, º)

O1—C1	1.207 (2)	C9—C14	1.375 (3)
O2—C8	1.199 (2)	C10—C11	1.384 (3)
O3—C10	1.360 (2)	C11—C12	1.381 (3)
O3—C15	1.420 (3)	C12—C13	1.363 (4)
N1—C1	1.3982 (19)	C13—C14	1.379 (3)
N1—C8	1.404 (2)	C3—H3	0.9300

N1—C9	1.422 (2)	C4—H4	0.9300
C1—C2	1.479 (2)	C5—H5	0.9300
C2—C3	1.376 (2)	C6—H6	0.9300
C2—C7	1.381 (2)	C11—H11	0.9300
C3—C4	1.384 (3)	C12—H12	0.9300
C4—C5	1.376 (3)	C13—H13	0.9300
C5—C6	1.382 (3)	C14—H14	0.9300
C6—C7	1.376 (2)	C15—H15A	0.9600
C7—C8	1.478 (2)	C15—H15B	0.9600
C9—C10	1.390 (3)	C15—H15C	0.9600

C10—O3—C15	118.01 (16)	C10—C11—C12	119.6 (2)
C1—N1—C8	111.45 (12)	C11—C12—C13	121.5 (2)
C1—N1—C9	124.67 (13)	C12—C13—C14	119.4 (2)
C8—N1—C9	123.82 (13)	C9—C14—C13	119.9 (2)
O1—C1—N1	124.79 (14)	C2—C3—H3	121.00
O1—C1—C2	129.10 (14)	C4—C3—H3	121.00
N1—C1—C2	106.07 (13)	C3—C4—H4	119.00
C1—C2—C3	130.67 (15)	C5—C4—H4	119.00
C1—C2—C7	108.06 (13)	C4—C5—H5	119.00
C3—C2—C7	121.19 (16)	C6—C5—H5	119.00
C2—C3—C4	117.39 (17)	C5—C6—H6	121.00
C3—C4—C5	121.29 (17)	C7—C6—H6	121.00
C4—C5—C6	121.32 (18)	C10—C11—H11	120.00
C5—C6—C7	117.27 (17)	C12—C11—H11	120.00
C2—C7—C6	121.50 (15)	C11—C12—H12	119.00
C2—C7—C8	108.70 (14)	C13—C12—H12	119.00
C6—C7—C8	129.79 (15)	C12—C13—H13	120.00
O2—C8—N1	125.14 (15)	C14—C13—H13	120.00
O2—C8—C7	129.26 (15)	C9—C14—H14	120.00
N1—C8—C7	105.59 (12)	C13—C14—H14	120.00
N1—C9—C10	119.79 (15)	O3—C15—H15A	110.00
N1—C9—C14	119.34 (18)	O3—C15—H15B	109.00
C10—C9—C14	120.86 (16)	O3—C15—H15C	109.00
O3—C10—C9	116.81 (15)	H15A—C15—H15B	109.00
O3—C10—C11	124.44 (18)	H15A—C15—H15C	109.00
C9—C10—C11	118.75 (17)	H15B—C15—H15C	109.00

C15—O3—C10—C9	174.12 (17)	C3—C2—C7—C6	1.9 (2)
C15—O3—C10—C11	−6.5 (3)	C3—C2—C7—C8	−179.07 (14)
C8—N1—C1—O1	−177.05 (15)	C2—C3—C4—C5	−1.5 (3)
C8—N1—C1—C2	0.97 (17)	C3—C4—C5—C6	1.7 (3)
C9—N1—C1—O1	0.1 (3)	C4—C5—C6—C7	−0.1 (3)
C9—N1—C1—C2	178.09 (16)	C5—C6—C7—C2	−1.7 (2)
C1—N1—C8—O2	−177.22 (15)	C5—C6—C7—C8	179.52 (17)
C1—N1—C8—C7	1.25 (17)	C2—C7—C8—O2	175.22 (16)
C9—N1—C8—O2	5.6 (3)	C2—C7—C8—N1	−3.16 (16)
C9—N1—C8—C7	−175.90 (15)	C6—C7—C8—O2	−5.9 (3)

C1—N1—C9—C10	71.9 (2)	C6—C7—C8—N1	175.74 (15)
C1—N1—C9—C14	−109.5 (2)	N1—C9—C10—O3	−1.6 (3)
C8—N1—C9—C10	−111.38 (19)	N1—C9—C10—C11	179.02 (17)
C8—N1—C9—C14	67.2 (3)	C14—C9—C10—O3	179.80 (18)
O1—C1—C2—C3	−1.9 (3)	C14—C9—C10—C11	0.4 (3)
O1—C1—C2—C7	174.92 (16)	N1—C9—C14—C13	−178.45 (19)
N1—C1—C2—C3	−179.77 (16)	C10—C9—C14—C13	0.2 (3)
N1—C1—C2—C7	−2.98 (16)	O3—C10—C11—C12	−179.6 (2)
C1—C2—C3—C4	176.14 (17)	C9—C10—C11—C12	−0.3 (3)
C7—C2—C3—C4	−0.3 (2)	C10—C11—C12—C13	−0.4 (4)
C1—C2—C7—C6	−175.24 (14)	C11—C12—C13—C14	1.0 (4)
C1—C2—C7—C8	3.77 (17)	C12—C13—C14—C9	−0.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.93	2.57	3.428 (2)	153
C12—H12···O2^{ii}	0.93	2.46	3.313 (2)	152

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