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N-(4-Methoxyphenyl)phthalimide

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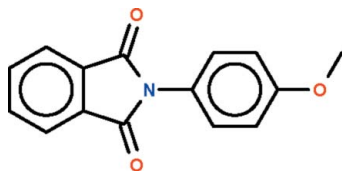
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 Key indicators: single-crystal X-ray study; $T = 123$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.039; wR factor = 0.104; data-to-parameter ratio = 15.3.

 The phthalimide fused-ring system and the phenylene ring in the title compound, $\text{C}_{15}\text{H}_{11}\text{NO}_3$, are inclined at an angle of 60.0 (1)°.

Related literature

 For the crystal structures of *N*-(phenyl)phthalimides, see: Izotova *et al.* (2009); Magomedova *et al.* (1980). For the 4-methyl-substituted derivative, see: Bocelli *et al.* (1995).


Experimental

Crystal data

 $\text{C}_{15}\text{H}_{11}\text{NO}_3$
 $M_r = 253.25$

 Monoclinic, $P2_1/c$
 $a = 18.6152$ (5) Å
 $b = 3.8502$ (1) Å
 $c = 16.3125$ (4) Å
 $\beta = 96.704$ (2)°
 $V = 1161.16$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 123$ K
 $0.40 \times 0.06 \times 0.04$ mm

Data collection

 Bruker SMART APEX
 diffractometer
 Absorption correction: none
 9965 measured reflections

 2645 independent reflections
 1927 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.104$
 $S = 1.01$
 2645 reflections

 173 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

 Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5040).

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supplementary materials

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N-(4-Methoxyphenyl)phthalimide

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Experimental

Phthalic anhydride (1.83 g, 12.4 mmol) and 4-methoxyaniline (1.01 g, 8.24 mmol) were heated in acetic acid (10 ml) for 4 h. The mixture was cooled and then was poured into water. The solid that separated was collected and recrystallized from ethanol in 60% yield.

Refinement

H-atoms were placed in calculated positions (C—H 0.95 or 0.98 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U(\text{C})$ or $1.5U(\text{C}_{\text{methyl}})$.

Figures

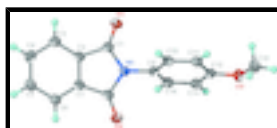


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of $\text{C}_{15}\text{H}_{11}\text{NO}_3$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

N-(4-Methoxyphenyl)phthalimide

Crystal data

$\text{C}_{15}\text{H}_{11}\text{NO}_3$	$F_{000} = 528$
$M_r = 253.25$	$D_x = 1.449 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ybc	Cell parameters from 2162 reflections
$a = 18.6152 (5) \text{ \AA}$	$\theta = 2.6\text{--}28.1^\circ$
$b = 3.8502 (1) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$c = 16.3125 (4) \text{ \AA}$	$T = 123 \text{ K}$
$\beta = 96.704 (2)^\circ$	Colorless, prism
$V = 1161.16 (5) \text{ \AA}^3$	$0.40 \times 0.06 \times 0.04 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART APEX diffractometer	1927 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.038$
Monochromator: graphite	$\theta_{\text{max}} = 27.5^\circ$
$T = 123 \text{ K}$	$\theta_{\text{min}} = 1.1^\circ$

supplementary materials

ω scans $h = -24 \rightarrow 24$
Absorption correction: None $k = -4 \rightarrow 4$
9965 measured reflections $l = -19 \rightarrow 21$
2645 independent reflections

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier map
Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites
 $R[F^2 > 2\sigma(F^2)] = 0.039$ H-atom parameters constrained
 $wR(F^2) = 0.104$ $w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 0.5469P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $S = 1.01$ $(\Delta/\sigma)_{\max} = 0.001$
2645 reflections $\Delta\rho_{\max} = 0.23 \text{ e } \text{\AA}^{-3}$
173 parameters $\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.23040 (7)	0.2003 (4)	0.30862 (8)	0.0191 (3)
O1	0.13566 (6)	0.4704 (3)	0.36518 (7)	0.0265 (3)
O2	0.29659 (6)	-0.0742 (3)	0.21493 (7)	0.0249 (3)
O3	0.44516 (6)	0.1734 (3)	0.57594 (7)	0.0240 (3)
C1	0.16067 (8)	0.3406 (4)	0.30709 (10)	0.0195 (3)
C2	0.12587 (8)	0.2999 (4)	0.22082 (10)	0.0187 (3)
C3	0.05760 (8)	0.3925 (4)	0.18527 (10)	0.0214 (4)
H3	0.0239	0.4996	0.2167	0.026*
C4	0.04005 (9)	0.3230 (4)	0.10160 (10)	0.0234 (4)
H4	-0.0068	0.3803	0.0756	0.028*
C5	0.08989 (9)	0.1710 (4)	0.05523 (10)	0.0236 (4)
H5	0.0768	0.1297	-0.0020	0.028*
C6	0.15867 (9)	0.0785 (4)	0.09164 (10)	0.0211 (4)
H6	0.1929	-0.0255	0.0603	0.025*
C7	0.17521 (8)	0.1437 (4)	0.17481 (10)	0.0185 (3)
C8	0.24232 (8)	0.0711 (4)	0.23055 (10)	0.0192 (3)
C9	0.28401 (8)	0.1935 (4)	0.37938 (10)	0.0191 (3)
C10	0.26872 (8)	0.0433 (4)	0.45236 (10)	0.0201 (3)
H10	0.2223	-0.0543	0.4559	0.024*
C11	0.32090 (8)	0.0343 (4)	0.52048 (10)	0.0206 (3)
H11	0.3102	-0.0641	0.5711	0.025*
C12	0.38907 (8)	0.1716 (4)	0.51360 (10)	0.0194 (3)
C13	0.40427 (8)	0.3237 (4)	0.44008 (10)	0.0213 (4)
H13	0.4509	0.4182	0.4360	0.026*
C14	0.35172 (8)	0.3369 (4)	0.37337 (10)	0.0211 (4)
H14	0.3617	0.4435	0.3234	0.025*

C15	0.43407 (9)	0.0139 (5)	0.65216 (10)	0.0255 (4)
H15A	0.4789	0.0251	0.6901	0.038*
H15B	0.4202	-0.2295	0.6424	0.038*
H15C	0.3955	0.1362	0.6764	0.038*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0191 (6)	0.0228 (7)	0.0162 (7)	0.0004 (5)	0.0050 (5)	-0.0009 (5)
O1	0.0258 (6)	0.0341 (7)	0.0207 (6)	0.0032 (5)	0.0080 (5)	-0.0052 (5)
O2	0.0225 (6)	0.0290 (7)	0.0244 (6)	0.0061 (5)	0.0075 (5)	-0.0012 (5)
O3	0.0214 (6)	0.0304 (7)	0.0197 (6)	-0.0022 (5)	0.0010 (5)	0.0021 (5)
C1	0.0199 (8)	0.0188 (8)	0.0210 (8)	-0.0010 (6)	0.0075 (6)	0.0012 (6)
C2	0.0217 (8)	0.0164 (8)	0.0191 (8)	-0.0019 (6)	0.0070 (6)	0.0010 (6)
C3	0.0208 (8)	0.0205 (8)	0.0243 (9)	0.0004 (6)	0.0082 (7)	0.0021 (7)
C4	0.0210 (8)	0.0231 (9)	0.0258 (9)	-0.0016 (7)	0.0021 (7)	0.0047 (7)
C5	0.0287 (9)	0.0231 (9)	0.0188 (8)	-0.0032 (7)	0.0022 (7)	0.0013 (7)
C6	0.0254 (8)	0.0193 (8)	0.0195 (8)	-0.0009 (7)	0.0066 (6)	-0.0001 (7)
C7	0.0212 (8)	0.0161 (8)	0.0194 (8)	-0.0021 (6)	0.0072 (6)	0.0019 (6)
C8	0.0226 (8)	0.0172 (8)	0.0190 (8)	-0.0014 (6)	0.0071 (6)	0.0010 (6)
C9	0.0200 (8)	0.0184 (8)	0.0191 (8)	0.0018 (6)	0.0032 (6)	-0.0019 (6)
C10	0.0194 (8)	0.0205 (8)	0.0213 (9)	-0.0021 (6)	0.0068 (6)	-0.0010 (6)
C11	0.0244 (8)	0.0202 (8)	0.0181 (8)	-0.0001 (6)	0.0064 (6)	0.0005 (6)
C12	0.0203 (8)	0.0174 (8)	0.0204 (8)	0.0023 (6)	0.0028 (6)	-0.0024 (6)
C13	0.0196 (8)	0.0217 (9)	0.0238 (9)	-0.0002 (7)	0.0075 (6)	-0.0003 (7)
C14	0.0237 (8)	0.0211 (8)	0.0200 (8)	-0.0004 (7)	0.0078 (6)	0.0012 (6)
C15	0.0291 (9)	0.0274 (10)	0.0196 (9)	-0.0009 (7)	0.0017 (7)	0.0022 (7)

Geometric parameters (\AA , $^\circ$)

N1—C1	1.4034 (19)	C6—C7	1.379 (2)
N1—C8	1.409 (2)	C6—H6	0.9500
N1—C9	1.435 (2)	C7—C8	1.483 (2)
O1—C1	1.2114 (19)	C9—C10	1.383 (2)
O2—C8	1.2080 (18)	C9—C14	1.390 (2)
O3—C12	1.3699 (19)	C10—C11	1.388 (2)
O3—C15	1.4232 (19)	C10—H10	0.9500
C1—C2	1.487 (2)	C11—C12	1.391 (2)
C2—C3	1.381 (2)	C11—H11	0.9500
C2—C7	1.389 (2)	C12—C13	1.393 (2)
C3—C4	1.392 (2)	C13—C14	1.377 (2)
C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.392 (2)	C14—H14	0.9500
C4—H4	0.9500	C15—H15A	0.9800
C5—C6	1.393 (2)	C15—H15B	0.9800
C5—H5	0.9500	C15—H15C	0.9800
C1—N1—C8	111.27 (13)	O2—C8—C7	128.56 (15)
C1—N1—C9	125.17 (13)	N1—C8—C7	106.11 (13)

supplementary materials

C8—N1—C9	123.54 (13)	C10—C9—C14	120.42 (15)
C12—O3—C15	118.08 (12)	C10—C9—N1	120.41 (14)
O1—C1—N1	125.74 (15)	C14—C9—N1	119.17 (14)
O1—C1—C2	128.24 (15)	C9—C10—C11	120.29 (14)
N1—C1—C2	106.02 (13)	C9—C10—H10	119.9
C3—C2—C7	121.28 (15)	C11—C10—H10	119.9
C3—C2—C1	130.39 (14)	C10—C11—C12	119.05 (15)
C7—C2—C1	108.33 (14)	C10—C11—H11	120.5
C2—C3—C4	117.47 (15)	C12—C11—H11	120.5
C2—C3—H3	121.3	O3—C12—C11	124.43 (14)
C4—C3—H3	121.3	O3—C12—C13	115.03 (14)
C3—C4—C5	121.23 (15)	C11—C12—C13	120.53 (15)
C3—C4—H4	119.4	C14—C13—C12	119.94 (14)
C5—C4—H4	119.4	C14—C13—H13	120.0
C4—C5—C6	120.88 (16)	C12—C13—H13	120.0
C4—C5—H5	119.6	C13—C14—C9	119.75 (15)
C6—C5—H5	119.6	C13—C14—H14	120.1
C7—C6—C5	117.48 (15)	C9—C14—H14	120.1
C7—C6—H6	121.3	O3—C15—H15A	109.5
C5—C6—H6	121.3	O3—C15—H15B	109.5
C6—C7—C2	121.64 (15)	H15A—C15—H15B	109.5
C6—C7—C8	130.11 (14)	O3—C15—H15C	109.5
C2—C7—C8	108.24 (14)	H15A—C15—H15C	109.5
O2—C8—N1	125.32 (15)	H15B—C15—H15C	109.5
C8—N1—C1—O1	-179.83 (16)	C9—N1—C8—C7	-177.28 (14)
C9—N1—C1—O1	-1.1 (3)	C6—C7—C8—O2	-2.9 (3)
C8—N1—C1—C2	-0.56 (17)	C2—C7—C8—O2	176.86 (16)
C9—N1—C1—C2	178.14 (14)	C6—C7—C8—N1	178.40 (16)
O1—C1—C2—C3	-0.9 (3)	C2—C7—C8—N1	-1.81 (17)
N1—C1—C2—C3	179.88 (16)	C1—N1—C9—C10	55.6 (2)
O1—C1—C2—C7	178.63 (16)	C8—N1—C9—C10	-125.84 (17)
N1—C1—C2—C7	-0.62 (17)	C1—N1—C9—C14	-125.02 (17)
C7—C2—C3—C4	0.1 (2)	C8—N1—C9—C14	53.5 (2)
C1—C2—C3—C4	179.55 (16)	C14—C9—C10—C11	0.1 (2)
C2—C3—C4—C5	-1.0 (2)	N1—C9—C10—C11	179.42 (14)
C3—C4—C5—C6	1.0 (3)	C9—C10—C11—C12	-1.4 (2)
C4—C5—C6—C7	-0.1 (2)	C15—O3—C12—C11	2.2 (2)
C5—C6—C7—C2	-0.9 (2)	C15—O3—C12—C13	-178.34 (14)
C5—C6—C7—C8	178.91 (16)	C10—C11—C12—O3	-179.02 (14)
C3—C2—C7—C6	0.9 (2)	C10—C11—C12—C13	1.6 (2)
C1—C2—C7—C6	-178.69 (14)	O3—C12—C13—C14	-179.87 (14)
C3—C2—C7—C8	-178.96 (14)	C11—C12—C13—C14	-0.4 (2)
C1—C2—C7—C8	1.49 (17)	C12—C13—C14—C9	-0.9 (2)
C1—N1—C8—O2	-177.28 (15)	C10—C9—C14—C13	1.1 (2)
C9—N1—C8—O2	4.0 (2)	N1—C9—C14—C13	-178.24 (14)
C1—N1—C8—C7	1.44 (17)		

Fig. 1

