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N-(4-Methoxyphenyl)phthalimide

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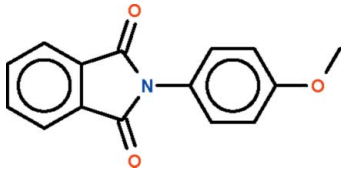
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.104; data-to-parameter ratio = 15.3.

The phthalimide fused-ring system and the phenylene ring in the title compound, $C_{15}H_{11}NO_3$, 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

$C_{15}H_{11}NO_3$ M_r = 253.25
Monoclinic, $P2_1/c$
a = 18.6152 (5) Å
b = 3.8502 (1) Å
c = 16.3125 (4) Å
β = 96.704 (2)°
V = 1161.16 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 123 K
0.40 × 0.06 × 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_{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
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −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).

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

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supporting information

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S1. 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.

S2. 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(H) set to 1.2U(C) or 1.5U(C_{methyl}).

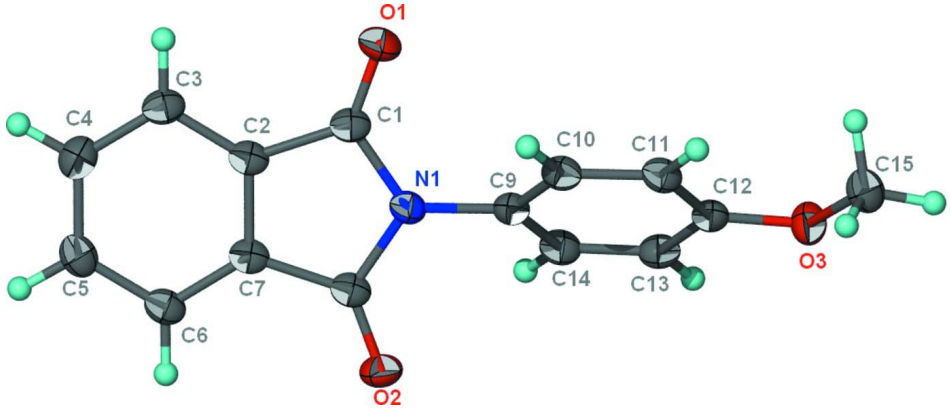

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{15}H_{11}NO_3$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

N-(4-Methoxyphenyl)phthalimide

Crystal data

$C_{15}H_{11}NO_3$
M_r = 253.25
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 18.6152 (5) Å
b = 3.8502 (1) Å
c = 16.3125 (4) Å
β = 96.704 (2)°
V = 1161.16 (5) Å^3
Z = 4
F(000) = 528
D_x = 1.449 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2162 reflections
θ = 2.6–28.1°
μ = 0.10 mm^{-1}
T = 123 K
Colorless, prism
0.40 × 0.06 × 0.04 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
9965 measured reflections
2645 independent reflections

1927 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.1°$
$h = -24 \rightarrow 24$
$k = -4 \rightarrow 4$
$l = -19 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.104$
$S = 1.01$
2645 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
$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 0.5469P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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 (Å, º)

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)
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)		