Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(2-Methoxyphenyl)phthalimide

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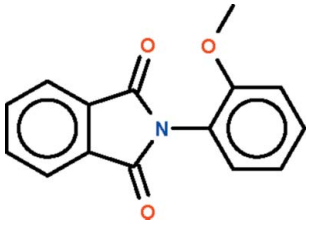
Received 17 August 2009; accepted 18 August 2009

Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.098; data-to-parameter ratio = 15.5.

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 54.2 (1)°.

Related literature

For the crystal structures of *N*-(phenyl)phthalimides, see: Izotova *et al.* (2009); Magomedova *et al.* (1980). For that of the 2-ethyl-substituted derivative, see: Fan *et al.* (2008).



Experimental

Crystal data

$C_{15}H_{11}NO_3$ M_r = 253.25
Monoclinic, $P2_1/n$
a = 11.8505 (2) Å
b = 6.6903 (1) Å
c = 15.3264 (3) Å
β = 106.258 (1)°
V = 1166.54 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 123 K
0.28 × 0.16 × 0.04 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
10672 measured reflections
2682 independent reflections
2190 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.098
S = 1.03
2682 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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: BT5039).

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supplementary materials

Acta Cryst. (2009). E**65**, o2218 [**doi:10.1107/S1600536809032826**]

N-(2-Methoxyphenyl)phthalimide

Y. L. Sim, A. Ariffin, M. N. Khan and S. W. Ng

Experimental

Phthalic anhydride (5.00 g, 33.8 mmol) and 4-methoxyaniline (4.99 g, 40.5 mmol) were heated in acetic acid (15 ml) for 4 h. The mixture was cooled and then poured into water. The solid that separated was collected and recrystallized from ethanol in 90% 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(H) set to 1.2 U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

Figures

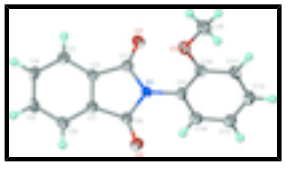

Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{15}H_{11}NO_3$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

N-(2-Methoxyphenyl)phthalimide

Crystal data

$C_{15}H_{11}NO_3$	F_{000} = 528
M_r = 253.25	D_x = 1.442 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3112 reflections
a = 11.8505 (2) Å	θ = 2.5–28.3º
b = 6.6903 (1) Å	μ = 0.10 mm^{-1}
c = 15.3264 (3) Å	T = 123 K
β = 106.258 (1)º	Irregular, colorless
V = 1166.54 (3) Å^3	0.28 × 0.16 × 0.04 mm
Z = 4	

Data collection

Bruker SMART APEX diffractometer	2190 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.028
Monochromator: graphite	θ_{max} = 27.5º

T = 123 K	θ_{min} = 1.9º
ω scans	h = −14→15
Absorption correction: None	k = −8→8
10672 measured reflections	l = −19→19
2682 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
$R[F^2 > 2\sigma(F^2)]$ = 0.036	H-atom parameters constrained
$wR(F^2)$ = 0.098	$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.3213P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
2682 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
173 parameters	$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.76144 (8)	0.26041 (14)	0.47272 (6)	0.0232 (2)
O2	0.74087 (8)	0.35172 (14)	0.76449 (6)	0.0242 (2)
O3	0.89049 (8)	0.63238 (14)	0.56474 (6)	0.0240 (2)
N1	0.78134 (9)	0.32357 (16)	0.62507 (7)	0.0183 (2)
C1	0.71795 (11)	0.28292 (18)	0.53464 (8)	0.0177 (3)
C2	0.59283 (11)	0.26801 (17)	0.53474 (8)	0.0168 (3)
C3	0.49248 (11)	0.23766 (18)	0.46394 (9)	0.0187 (3)
H3	0.4962	0.2240	0.4031	0.022*
C4	0.38571 (11)	0.22777 (19)	0.48501 (9)	0.0205 (3)
H4	0.3149	0.2111	0.4376	0.025*
C5	0.38127 (11)	0.24202 (19)	0.57471 (9)	0.0227 (3)
H5	0.3075	0.2333	0.5875	0.027*
C6	0.48287 (11)	0.26884 (19)	0.64603 (9)	0.0203 (3)
H6	0.4801	0.2758	0.7073	0.024*
C7	0.58786 (11)	0.28491 (18)	0.62405 (8)	0.0178 (3)
C8	0.70848 (11)	0.32285 (18)	0.68350 (8)	0.0180 (3)
C9	0.90625 (10)	0.34589 (19)	0.65589 (8)	0.0183 (3)
C10	0.96165 (11)	0.50402 (19)	0.62429 (8)	0.0187 (3)
C11	1.08374 (11)	0.5197 (2)	0.65517 (8)	0.0226 (3)
H11	1.1233	0.6222	0.6324	0.027*
C12	1.14739 (12)	0.3852 (2)	0.71924 (9)	0.0251 (3)
H12	1.2304	0.3983	0.7409	0.030*
C13	1.09199 (12)	0.2325 (2)	0.75213 (9)	0.0242 (3)
H13	1.1362	0.1429	0.7968	0.029*
C14	0.97095 (11)	0.2121 (2)	0.71899 (9)	0.0217 (3)

H14	0.9323	0.1054	0.7398	0.026*
C15	0.94409 (12)	0.8082 (2)	0.54130 (10)	0.0254 (3)
H15A	0.9847	0.8806	0.5968	0.038*
H15B	0.8835	0.8942	0.5026	0.038*
H15C	1.0009	0.7703	0.5084	0.038*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0218 (5)	0.0299 (5)	0.0200 (5)	−0.0019 (4)	0.0091 (4)	−0.0012 (4)
O2	0.0228 (5)	0.0319 (5)	0.0176 (5)	−0.0004 (4)	0.0051 (4)	−0.0019 (4)
O3	0.0189 (5)	0.0231 (5)	0.0292 (5)	−0.0019 (4)	0.0052 (4)	0.0068 (4)
N1	0.0151 (5)	0.0223 (6)	0.0175 (5)	−0.0013 (4)	0.0047 (4)	0.0012 (4)
C1	0.0196 (6)	0.0152 (6)	0.0183 (6)	−0.0002 (4)	0.0054 (5)	0.0018 (5)
C2	0.0174 (6)	0.0138 (6)	0.0199 (6)	0.0000 (4)	0.0066 (5)	0.0019 (4)
C3	0.0211 (6)	0.0160 (6)	0.0187 (6)	0.0010 (5)	0.0049 (5)	0.0006 (5)
C4	0.0173 (6)	0.0180 (6)	0.0240 (6)	0.0000 (5)	0.0019 (5)	0.0002 (5)
C5	0.0176 (6)	0.0235 (7)	0.0282 (7)	−0.0013 (5)	0.0084 (5)	−0.0013 (5)
C6	0.0198 (6)	0.0220 (7)	0.0205 (6)	−0.0007 (5)	0.0079 (5)	−0.0001 (5)
C7	0.0196 (6)	0.0151 (6)	0.0186 (6)	−0.0006 (5)	0.0053 (5)	0.0005 (5)
C8	0.0182 (6)	0.0161 (6)	0.0201 (6)	0.0010 (5)	0.0063 (5)	0.0017 (5)
C9	0.0148 (6)	0.0226 (6)	0.0177 (6)	−0.0009 (5)	0.0047 (5)	−0.0025 (5)
C10	0.0186 (6)	0.0209 (6)	0.0174 (6)	0.0003 (5)	0.0061 (5)	−0.0016 (5)
C11	0.0193 (6)	0.0259 (7)	0.0242 (6)	−0.0044 (5)	0.0089 (5)	−0.0016 (5)
C12	0.0155 (6)	0.0337 (8)	0.0256 (7)	−0.0005 (5)	0.0050 (5)	−0.0022 (6)
C13	0.0206 (7)	0.0296 (7)	0.0217 (6)	0.0042 (5)	0.0045 (5)	0.0029 (5)
C14	0.0214 (7)	0.0237 (7)	0.0212 (6)	0.0004 (5)	0.0080 (5)	0.0016 (5)
C15	0.0270 (7)	0.0205 (7)	0.0296 (7)	−0.0032 (5)	0.0097 (6)	0.0032 (5)

Geometric parameters (Å, °)

O1—C1	1.2095 (15)	C6—C7	1.3812 (18)
O2—C8	1.2077 (15)	C6—H6	0.9500
O3—C10	1.3604 (15)	C7—C8	1.4862 (17)
O3—C15	1.4296 (16)	C9—C14	1.3818 (18)
N1—C1	1.4057 (16)	C9—C10	1.4010 (18)
N1—C8	1.4073 (16)	C10—C11	1.3946 (17)
N1—C9	1.4301 (15)	C11—C12	1.3885 (19)
C1—C2	1.4865 (17)	C11—H11	0.9500
C2—C3	1.3821 (17)	C12—C13	1.383 (2)
C2—C7	1.3910 (17)	C12—H12	0.9500
C3—C4	1.3923 (18)	C13—C14	1.3879 (18)
C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.3937 (18)	C14—H14	0.9500
C4—H4	0.9500	C15—H15A	0.9800
C5—C6	1.3927 (18)	C15—H15B	0.9800
C5—H5	0.9500	C15—H15C	0.9800
C10—O3—C15	116.90 (10)	O2—C8—C7	129.18 (12)

C1—N1—C8	111.90 (10)	N1—C8—C7	105.46 (10)
C1—N1—C9	124.33 (10)	C14—C9—C10	120.61 (11)
C8—N1—C9	123.56 (10)	C14—C9—N1	118.93 (11)
O1—C1—N1	124.77 (12)	C10—C9—N1	120.43 (11)
O1—C1—C2	129.54 (11)	O3—C10—C11	124.71 (11)
N1—C1—C2	105.66 (10)	O3—C10—C9	116.50 (11)
C3—C2—C7	121.35 (11)	C11—C10—C9	118.79 (11)
C3—C2—C1	130.42 (11)	C12—C11—C10	119.85 (12)
C7—C2—C1	108.21 (11)	C12—C11—H11	120.1
C2—C3—C4	117.57 (12)	C10—C11—H11	120.1
C2—C3—H3	121.2	C13—C12—C11	121.12 (12)
C4—C3—H3	121.2	C13—C12—H12	119.4
C3—C4—C5	120.89 (12)	C11—C12—H12	119.4
C3—C4—H4	119.6	C12—C13—C14	119.12 (12)
C5—C4—H4	119.6	C12—C13—H13	120.4
C6—C5—C4	121.32 (12)	C14—C13—H13	120.4
C6—C5—H5	119.3	C9—C14—C13	120.42 (12)
C4—C5—H5	119.3	C9—C14—H14	119.8
C7—C6—C5	117.29 (12)	C13—C14—H14	119.8
C7—C6—H6	121.4	O3—C15—H15A	109.5
C5—C6—H6	121.4	O3—C15—H15B	109.5
C6—C7—C2	121.53 (11)	H15A—C15—H15B	109.5
C6—C7—C8	129.88 (12)	O3—C15—H15C	109.5
C2—C7—C8	108.59 (11)	H15A—C15—H15C	109.5
O2—C8—N1	125.34 (11)	H15B—C15—H15C	109.5
C8—N1—C1—O1	−174.23 (12)	C9—N1—C8—C7	−176.91 (11)
C9—N1—C1—O1	0.68 (19)	C6—C7—C8—O2	−1.5 (2)
C8—N1—C1—C2	3.86 (13)	C2—C7—C8—O2	177.74 (13)
C9—N1—C1—C2	178.77 (11)	C6—C7—C8—N1	179.86 (12)
O1—C1—C2—C3	−4.7 (2)	C2—C7—C8—N1	−0.90 (13)
N1—C1—C2—C3	177.31 (12)	C1—N1—C9—C14	−117.21 (13)
O1—C1—C2—C7	173.64 (12)	C8—N1—C9—C14	57.11 (17)
N1—C1—C2—C7	−4.33 (13)	C1—N1—C9—C10	64.41 (16)
C7—C2—C3—C4	1.02 (18)	C8—N1—C9—C10	−121.27 (13)
C1—C2—C3—C4	179.20 (12)	C15—O3—C10—C11	−7.96 (18)
C2—C3—C4—C5	−1.90 (18)	C15—O3—C10—C9	172.06 (11)
C3—C4—C5—C6	0.75 (19)	C14—C9—C10—O3	−177.71 (11)
C4—C5—C6—C7	1.31 (19)	N1—C9—C10—O3	0.64 (17)
C5—C6—C7—C2	−2.21 (19)	C14—C9—C10—C11	2.31 (18)
C5—C6—C7—C8	176.94 (12)	N1—C9—C10—C11	−179.34 (11)
C3—C2—C7—C6	1.07 (19)	O3—C10—C11—C12	177.10 (12)
C1—C2—C7—C6	−177.47 (11)	C9—C10—C11—C12	−2.92 (19)
C3—C2—C7—C8	−178.24 (11)	C10—C11—C12—C13	1.2 (2)
C1—C2—C7—C8	3.22 (13)	C11—C12—C13—C14	1.2 (2)
C1—N1—C8—O2	179.33 (12)	C10—C9—C14—C13	0.07 (19)
C9—N1—C8—O2	4.38 (19)	N1—C9—C14—C13	−178.31 (11)
C1—N1—C8—C7	−1.96 (13)	C12—C13—C14—C9	−1.8 (2)

Fig. 1