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# *N*-(2-Methoxyphenyl)phthalimide

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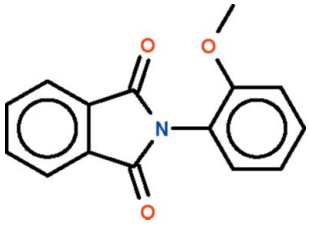
Key indicators: single-crystal X-ray study; $T$ = 123 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.098; data-to-parameter ratio = 15.5.

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
$\beta$ = 106.258 (1)°
$V$ = 1166.54 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 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).

## References

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# supporting information

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

## *N*-(2-Methoxyphenyl)phthalimide

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### S1. 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.

### 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 1.2 $U_{eq}$(C) or 1.5$U_{eq}$($C_{methyl}$).

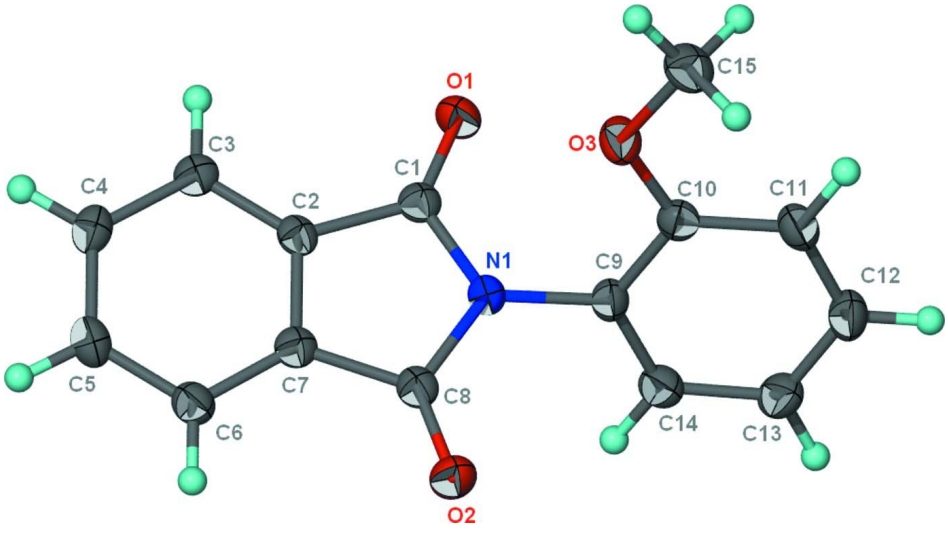


**Figure 1**

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*-(2-Methoxyphenyl)phthalimide

*Crystal data*

$C_{15}H_{11}NO_3$
$M_r$ = 253.25
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 11.8505 (2) Å
$b$ = 6.6903 (1) Å
$c$ = 15.3264 (3) Å
$\beta$ = 106.258 (1)°
$V$ = 1166.54 (3) Å$^3$
$Z$ = 4
$F$(000) = 528
$D_x$ = 1.442 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 3112 reflections
$\theta$ = 2.5–28.3°
$\mu$ = 0.10 mm$^{-1}$

$T$ = 123 K
Irregular, colorless

0.28 × 0.16 × 0.04 mm

*Data collection*

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
10672 measured reflections
2682 independent reflections

2190 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 1.9°
$h$ = −14→15
$k$ = −8→8
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.098
$S$ = 1.03
2682 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
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.3213P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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) |