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N-(3-Bromophenyl)phthalimide

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Key indicators

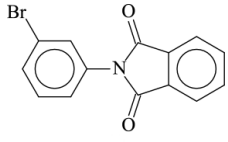
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.036
wR factor = 0.075
Data-to-parameter ratio = 12.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The benzene and phthalimido portions of the molecule of *N*-(3-bromophenyl)phthalimide, $C_{14}H_8BrNO_2$, are twisted by 38.1 (1) Å; two molecules are linked across a center of inversion by Br···O interactions of length 3.093 (3) Å.

Comment

In the crystal structure of *N*-(2-bromophenyl)phthalimide, (I), the benzene and phthalimide portions of the molecule are almost perpendicular to each other; the structure features an intermolecular Br···O contact of about 3.1 Å that is interpreted in terms of possible charge-transfer or dipole–dipole interactions (Wu *et al.*, 2002). The two portions are twisted by 38.1 (1)° in the present 3-bromo analog (Fig. 1), which also features a similar intermolecular interaction of 3.093 (3) Å (Fig. 2).



(I)

Experimental

Phthalic anhydride (5 g, 30 mmol) and 3-bromoaniline (3.7 ml, 30 mmol) were heated in ethanol (100 ml) for 2 h. The solution was filtered; slow cooling of the solution yielded the impure compound, which was then purified by recrystallization from ethanol (m.p. 421–423 K).

Crystal data

$C_{14}H_8BrNO_2$
M_r = 302.12
Monoclinic, $P2_1/n$
a = 12.025 (1) Å
b = 7.877 (1) Å
c = 12.877 (1) Å
β = 106.03 (1)°
V = 1172.3 (1) Å^3
Z = 4
D_x = 1.712 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 5.4–12.5°
μ = 3.50 mm^{-1}
T = 298 (2) K
Block, colorless
0.4 × 0.4 × 0.3 mm

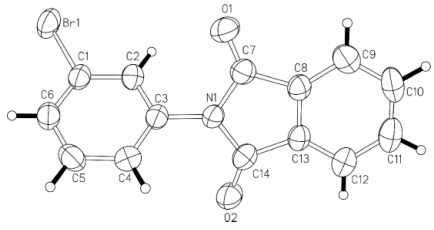


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: empirical *via* ψ scan (North *et al.*, 1968)
T_{min} = 0.269, T_{max} = 0.350
2160 measured reflections
2054 independent reflections
1433 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.0°
$h = 0 \rightarrow 14$
$k = -9 \rightarrow 0$
$l = -15 \rightarrow 14$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.075
S = 0.99
2054 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 0.8453P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0194 (10)

Table 1
Selected geometric parameters (Å, °).

Br1—C1	1.899 (4)	C4—C5	1.387 (5)
O1—C7	1.196 (4)	C5—C6	1.375 (5)
O2—C14	1.201 (4)	C7—C8	1.489 (5)
N1—C14	1.400 (4)	C8—C13	1.377 (5)
N1—C7	1.411 (4)	C8—C9	1.377 (5)
N1—C3	1.433 (4)	C9—C10	1.387 (5)
C1—C6	1.365 (5)	C10—C11	1.372 (6)
C1—C2	1.380 (4)	C11—C12	1.388 (5)
C2—C3	1.375 (5)	C12—C13	1.379 (5)
C3—C4	1.376 (5)	C13—C14	1.486 (5)
C14—N1—C3	124.9 (3)	N1—C7—C8	105.0 (3)
C14—N1—C7	112.3 (3)	C7—C8—C9	129.9 (4)
C3—N1—C7	122.8 (3)	C7—C8—C13	108.5 (3)
C2—C1—C6	121.8 (3)	C9—C8—C13	121.6 (3)
C6—C1—Br1	119.3 (3)	C8—C9—C10	117.2 (4)
C2—C1—Br1	118.9 (3)	C9—C10—C11	121.1 (4)
C1—C2—C3	118.4 (3)	C10—C11—C12	121.7 (4)
C2—C3—C4	121.3 (3)	C11—C12—C13	116.8 (4)
C2—C3—N1	118.9 (3)	C12—C13—C8	121.6 (3)
C4—C3—N1	119.8 (3)	C12—C13—C14	129.4 (3)
C3—C4—C5	118.7 (3)	C8—C13—C14	109.0 (3)
C4—C5—C6	120.9 (4)	O2—C14—N1	125.5 (3)
C1—C6—C5	118.9 (3)	O2—C14—C13	129.4 (3)
O1—C7—N1	125.5 (3)	N1—C14—C13	105.1 (3)
O1—C7—C8	129.5 (3)		

H atoms were placed at calculated positions [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$] and were refined using a riding model.

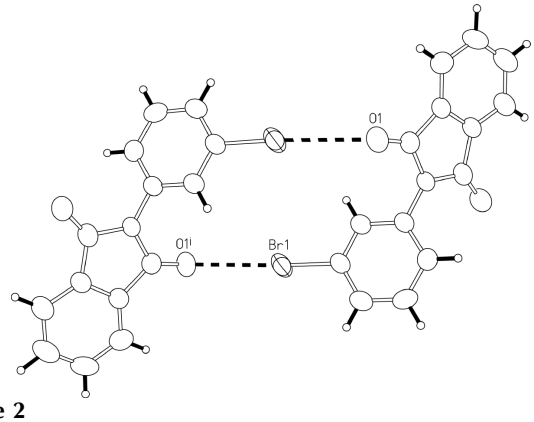


Figure 2
*ORTEP*II (Johnson, 1976) plot of (I), illustrating the Br···O interactions as dashed lines [symmetry code: (i) $1 - x, -y, 1 - z$].

Data collection: *CAD*-4/*PC* (Kretschmar, 1994); cell refinement: *CAD*-4 *VAX/PC Fortran System* (Enraf–Nonius, 1988); data reduction: *XCAD*4 (Harms, 1997) in *WinGX* (Farrugia, 1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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