

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

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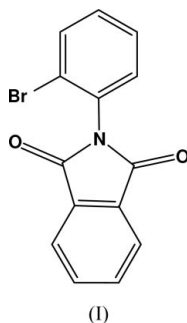
### Key indicators

Single-crystal X-ray study  
*T* = 298 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$   
*R* factor = 0.068  
*wR* factor = 0.054  
Data-to-parameter ratio = 11.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound,  $\text{C}_{14}\text{H}_8\text{BrNO}_2$ , was obtained as an *N*-protected starting material for the syntheses of multi-dentate ligands bearing *N*-donor atoms. Its crystal structure is reported here. The structure contains two orthogonal planar moieties (the bromophenyl ring and the phthalimide plane), with an interplanar angle of  $79.2(4)^\circ$ . A short intermolecular  $\text{Br}\cdots\text{O}$  distance of  $3.070(4) \text{ \AA}$  is observed.

### Comment

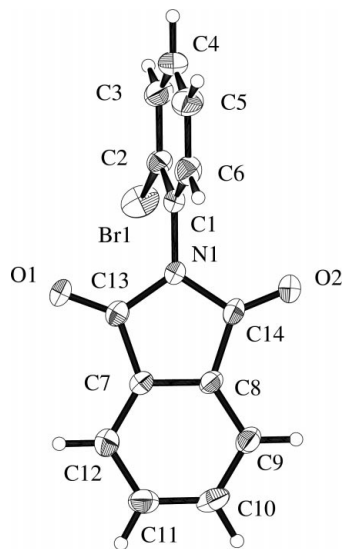
The crystal structure of *N*-(2-bromophenyl)phthalimide, (I), contains two almost perpendicular planar moieties, with an interplanar angle of  $79.2(?)^\circ$ . The bromophenyl and phthalimide rings are each essentially planar, within  $0.008 \text{ \AA}$ . All intramolecular distances are comparable to other aryl-phthalimide structures (Ribar *et al.*, 1976; Voliotis *et al.*, 1984). The short  $\text{Br}\cdots\text{O}$  distance of  $3.07(?) \text{ \AA}$  is shorter than the sum of van der Waals radii ( $1.85 + 1.52 \text{ \AA}$ ), but longer than some other reported  $\text{Br}\cdots\text{O}$  contact distances (Doi *et al.*, 1985). This short  $\text{Br}\cdots\text{O}$  contact indicates a possible charge-transfer interaction or dipole-dipole interaction between the Br atom and the carbonyl O atom. The relatively low C–C bond precision is probably due to the high proportion of weak data [only 46.5% greater than  $3\sigma(I)$ ].



### Experimental

The title compound, *N*-(2-bromophenyl)phthalimide, was obtained by adding phthalic anhydride (17.60 g) to liquid 2-bromoaniline (20.43 g) in a 1:1 molar ratio. The reaction mixture was heated with stirring until all the solid had dissolved (or reacted), and the temperature was maintained for approximately another 8 h. Cooling to room temperature led to a solidified product. Colorless crystals were obtained from a mixed solvent system of *n*-hexane and dichloromethane. The structure was supported by EI-MS ( $M^+ = 302$ ). The C, H, N and O contents were analysed using a Heraeus CHN–O instrument. Analysis calculated for  $\text{C}_{14}\text{H}_8\text{BrNO}_2$ : C 55.66, H 2.67, N 4.64, O 10.59%; found: C 55.26, H 2.70, N 4.68, O 10.55%.

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**Figure 1**  
A view of the molecule of the title compound, with 30% probability ellipsoids.

#### Crystal data

$C_{14}H_8BrNO_2$   
 $M_r = 302.11$   
 Monoclinic,  $P2_1/n$   
 $a = 11.330$  (1) Å  
 $b = 8.100$  (1) Å  
 $c = 13.965$  (1) Å  
 $\beta = 104.096$  (9)°  
 $V = 1243.0$  (2) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.614$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 19 reflections  
 $\theta = 5.4$ – $7.8^\circ$   
 $\mu = 3.30$  mm<sup>-1</sup>  
 $T = 298.2$  K  
 Prism, colorless  
 $0.60 \times 0.56 \times 0.48$  mm

#### Data collection

Rigaku AFC-7S diffractometer  
 $\omega$ - $2\theta$  scans  
 Absorption correction:  $\psi$  scans  
 (North *et al.*, 1968)  
 $T_{\min} = 0.155$ ,  $T_{\max} = 0.200$   
 3208 measured reflections  
 2852 independent reflections  
 1882 reflections with  $I > \sigma(I)$

$R_{\text{int}} = 0.059$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = 0 \rightarrow 14$   
 $k = 0 \rightarrow 10$   
 $l = -18 \rightarrow 17$   
 3 standard reflections  
 every 150 reflections  
 intensity decay:  $-0.2\%$

#### Refinement

Refinement on  $F$   
 $R = 0.068$   
 $wR = 0.054$   
 $S = 1.83$   
 1882 reflections  
 163 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o) + 0.00022|F_o|^2]$   
 $(\Delta/\sigma)_{\text{max}} = 0.007$   
 $\Delta\rho_{\text{max}} = 0.78$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.73$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Br1—C2	1.885 (4)	C4—C5	1.354 (8)
O1—C13	1.207 (5)	C5—C6	1.375 (7)
O2—C14	1.198 (5)	C7—C8	1.388 (6)
N1—C1	1.434 (5)	C7—C12	1.378 (6)
N1—C13	1.405 (6)	C7—C13	1.470 (6)
N1—C14	1.409 (5)	C8—C9	1.377 (6)
C1—C2	1.382 (6)	C8—C14	1.475 (7)
C1—C6	1.387 (6)	C9—C10	1.384 (7)
C2—C3	1.381 (6)	C10—C11	1.381 (7)
C3—C4	1.377 (7)	C11—C12	1.386 (7)
C1—N1—C13	124.5 (3)	C12—C7—C13	130.7 (4)
C1—N1—C14	124.2 (4)	C7—C8—C9	122.1 (4)
C13—N1—C14	111.4 (4)	C7—C8—C14	108.5 (4)
N1—C1—C2	121.0 (4)	C9—C8—C14	129.4 (4)
N1—C1—C6	119.0 (4)	C8—C9—C10	116.8 (4)
C2—C1—C6	119.9 (4)	C9—C10—C11	121.7 (4)
Br1—C2—C1	121.1 (3)	C10—C11—C12	121.0 (5)
Br1—C2—C3	119.7 (4)	C7—C12—C11	117.7 (4)
C1—C2—C3	119.2 (4)	O1—C13—N1	124.7 (4)
C2—C3—C4	120.3 (5)	O1—C13—C7	129.4 (4)
C3—C4—C5	120.3 (5)	N1—C13—C7	105.9 (4)
C4—C5—C6	120.6 (5)	O2—C14—N1	124.1 (4)
C1—C6—C5	119.7 (4)	O2—C14—C8	130.2 (4)
C8—C7—C12	120.7 (4)	N1—C14—C8	105.7 (4)
C8—C7—C13	108.6 (4)		

Phenyl H atoms were placed in calculated positions, with a C—H distance of 0.95 Å. All H atoms were included in the final cycles of least-squares refinement with fixed positional parameters and isotropic displacement parameters ( $1.2U_{\text{eq}}$  of the attached non-H atoms).

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1992–1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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#### References

- Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.  
 Doi, M., Yasuda, N., Ishida, T. & Inoue, M. (1985). *Chem. Pharm. Bull.* **33**, 2183–2189.  
 Molecular Structure Corporation (1992). *MSC/AFC Diffractometer Control Software*. Version 5.32. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.  
 Molecular Structure Corporation (1992–1997). *TEXSAN*. Version 1.7. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.  
 North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.  
 Ribar, B., Stenkovic, S. & Halasi, R. (1976). *Cryst. Struct. Commun.* **5**, 919–922.  
 Voliotis, S., Arrieta, J. M. & Germain, G. (1984). *Acta Cryst.* **C40**, 1946–1948.