

## 2-(4-Bromophenyl)quinoxaline

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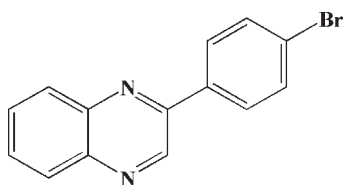
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Key indicators: single-crystal X-ray study;  $T = 153$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.032;  $wR$  factor = 0.075; data-to-parameter ratio = 17.3.

In the title compound,  $\text{C}_{14}\text{H}_9\text{BrN}_2$ , the benzene and quinoxaline rings are almost coplanar [r.m.s. deviation = 0.0285 (3) Å and dihedral angle = 2.1 (2)°].

### Related literature

For the synthesis of quinoxaline derivatives, see: Raw *et al.* (2003); Bhosale *et al.* (2005). For their applications, see: Brock *et al.* (1999); Seitz *et al.* (2002); He *et al.* (2003). For typical bond lengths in a related structure, see: Rong *et al.* (2006).



### Experimental

#### Crystal data

$\text{C}_{14}\text{H}_9\text{BrN}_2$   
 $M_r = 285.14$   
Monoclinic,  $P2_1/c$   
 $a = 13.959$  (3) Å  
 $b = 5.9031$  (12) Å

$c = 14.497$  (3) Å  
 $\beta = 109.53$  (3)°  
 $V = 1125.9$  (4) Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation

$\mu = 3.63$  mm<sup>-1</sup>  
 $T = 153$  K

0.20 × 0.18 × 0.10 mm

#### Data collection

Rigaku MM-007/Saturn 70 CCD  
area-detector diffractometer  
Absorption correction: multi-scan  
(*REQAB*; Jacobson, 1998)  
 $T_{\min} = 0.531$ ,  $T_{\max} = 0.713$

8910 measured reflections  
2683 independent reflections  
1763 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.052$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.075$   
 $S = 0.96$   
2683 reflections

155 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.76$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.69$  e Å<sup>-3</sup>

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2039).

### References

- Bhosale, R. S., Sarda, S. R., Ardhpure, S. S., Jadhav, W. N., Bhusare, S. R. & Pawar, R. P. (2005). *Tetrahedron Lett.* **46**, 7183–7186.
- Brock, E. D., Lewis, D. M., Yousaf, T. I. & Harper, H. H. (1999). (The Procter & Gamble Company, USA), World Patent WO 9 951 688.
- He, W., Myers, M. R., Hanney, B., Spada, A. P., Bilder, G., Galzinski, H., Amin, D., Needle, S., Page, K., Jayyosi, Z. & Perrone, M. H. (2003). *Bioorg. Med. Chem. Lett.* **13**, 3097–3100.
- Jacobson, R. (1998). *REQAB*. Private communication to the Rigaku Corporation, Tokyo, Japan.
- Raw, S. A., Wilfred, C. D. & Taylor, R. J. K. (2003). *Chem. Commun.* pp. 2286–2287.
- Rigaku/MSC (2005). *CrystalClear*. MSC, The Woodlands, Texas, USA, and Rigaku Corporation, Tokyo, Japan.
- Rong, L.-C., Li, X.-Y., Yao, C.-S., Wang, H.-Y. & Shi, D.-Q. (2006). *Acta Cryst. E62*, o1959–o1960.
- Seitz, L. E., Suling, W. J. & Reynolds, R. C. (2002). *J. Med. Chem.* **45**, 5604–5606.
- Sheldrick, G. M. (2008). *Acta Cryst. A64*, 112–122.

**supplementary materials**

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## 2-(4-Bromophenyl)quinoxaline

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### Comment

Quinoxaline derivatives are an important class of nitrogen containing heterocycles, finding use as intermediates in organic synthesis and in addition have been reported as having applications as anticancer, antiviral, and antibacterial agents (Seitz *et al.*, 2002; He *et al.*, 2003) and dyes (Brock *et al.*, 1999). In recent years, many syntheses of quinoxaline derivatives have been reported (Raw *et al.*, 2003; Bhosale *et al.*, 2005). The title compound  $C_{14}H_9BrN_2$  (I) is one of such quinoxaline derivatives which we have synthesized and now report its crystal structure.

The molecular structure of title compound is as shown in Fig.1. The bond lengths and angles are usual for this type of compound (Rong *et al.*, 2006). The dihedral angle between the benzene ring and quinoxaline ring is  $2.1(2)^\circ$ , which means that the benzene ring and the quinoxaline ring are approximately coplanar with a r.m.s deviation of  $0.0285(3) \text{ \AA}$ , the Br atom lying in the plane of the substituent benzene ring [r.m.s deviation,  $0.0271(3) \text{ \AA}$ ]. The crystal packing (Fig. 2) is stabilized by van der Waals forces.

### Experimental

A suspension of hydrated 2-(4-bromophenyl)-2-oxoacetaldehyde (2.0 mmol) and benzene-1,2-diamine (3.0 mmol) in ethanol (5 ml) was stirred at room temperature with the reaction progress monitored *via* TLC. The resulting precipitate was filtered off, washed with cold ethanol, dried and purified to give the title compound as a light yellow solid (92.5% yield: m.p. 418 K). Crystals suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform-ethanol (1:1).

### Refinement

All H atoms were positioned geometrically and refined as riding with  $C-H = 0.95 \text{ \AA}$  and  $U_{iso}(H)$  set equal to  $1.2U_{eq}(\text{carrier atom})$ .

### Figures

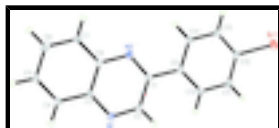


Fig. 1. Molecular configuration of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

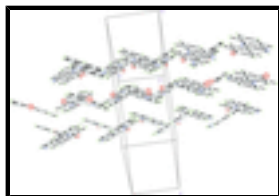


Fig. 2. The crystal packing of (I), viewed down the *c* axis.

## 2-(4-Bromophenyl)quinoxaline

### Crystal data

$C_{14}H_9BrN_2$	$F(000) = 568$
$M_r = 285.14$	$D_x = 1.682 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Melting point: 418 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 13.959 (3) \text{ \AA}$	Cell parameters from 3221 reflections
$b = 5.9031 (12) \text{ \AA}$	$\theta = 2.9\text{--}27.9^\circ$
$c = 14.497 (3) \text{ \AA}$	$\mu = 3.63 \text{ mm}^{-1}$
$\beta = 109.53 (3)^\circ$	$T = 153 \text{ K}$
$V = 1125.9 (4) \text{ \AA}^3$	Prism, colorless
$Z = 4$	$0.20 \times 0.18 \times 0.10 \text{ mm}$

### Data collection

Rigaku <b>Model name?</b> CCD area-detector diffractometer	2683 independent reflections
Radiation source: rotating anode multilayer	1763 reflections with $I > 2\sigma(I)$
Detector resolution: $7.31 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.052$
$\varphi$ and $\omega$ scans	$\theta_{\text{max}} = 27.9^\circ$ , $\theta_{\text{min}} = 2.9^\circ$
Absorption correction: multi-scan ( <i>REQAB</i> ; Jacobson, 1998)	$h = -18 \rightarrow 11$
$T_{\text{min}} = 0.531$ , $T_{\text{max}} = 0.713$	$k = -7 \rightarrow 7$
8910 measured reflections	$l = -19 \rightarrow 19$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.075$	$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2]$
$S = 0.96$	where $P = (F_o^2 + 2F_c^2)/3$
2683 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
155 parameters	$\Delta\rho_{\text{max}} = 0.76 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.69 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0540 (17)

*Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.460263 (18)	1.10538 (4)	0.33474 (2)	0.03213 (13)
N1	-0.12149 (15)	0.6560 (3)	0.02060 (15)	0.0218 (5)
N2	-0.05847 (15)	1.0700 (3)	0.12055 (14)	0.0169 (4)
C1	0.00712 (17)	0.9095 (4)	0.11986 (16)	0.0150 (5)
C2	-0.02653 (17)	0.7012 (4)	0.07034 (17)	0.0210 (6)
H2	0.0229	0.5882	0.0736	0.025*
C3	-0.19054 (16)	0.8203 (4)	0.02054 (16)	0.0160 (5)
C4	-0.29514 (17)	0.7808 (4)	-0.02863 (17)	0.0204 (6)
H4	-0.3168	0.6436	-0.0636	0.024*
C5	-0.36496 (18)	0.9398 (4)	-0.02576 (17)	0.0213 (6)
H5	-0.4352	0.9126	-0.0588	0.026*
C6	-0.33379 (19)	1.1438 (4)	0.02573 (18)	0.0229 (6)
H6	-0.3833	1.2523	0.0279	0.028*
C7	-0.23291 (17)	1.1877 (4)	0.07274 (17)	0.0176 (5)
H7	-0.2126	1.3275	0.1060	0.021*
C8	-0.15888 (16)	1.0252 (4)	0.07190 (15)	0.0150 (5)
C9	0.11683 (17)	0.9532 (4)	0.17107 (16)	0.0157 (5)
C10	0.19145 (17)	0.7987 (4)	0.16884 (17)	0.0186 (5)
H10	0.1721	0.6609	0.1337	0.022*
C11	0.29343 (17)	0.8427 (4)	0.21702 (18)	0.0206 (6)
H11	0.3437	0.7360	0.2152	0.025*
C12	0.32117 (17)	1.0434 (4)	0.26773 (17)	0.0186 (5)
C13	0.24914 (17)	1.2017 (4)	0.27042 (17)	0.0196 (5)
H13	0.2692	1.3406	0.3045	0.023*
C14	0.14782 (18)	1.1554 (4)	0.22297 (16)	0.0186 (5)
H14	0.0980	1.2627	0.2255	0.022*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.01429 (15)	0.0399 (2)	0.03931 (19)	-0.00711 (11)	0.00519 (12)	-0.00733 (13)
N1	0.0176 (11)	0.0191 (10)	0.0248 (11)	0.0017 (8)	0.0021 (9)	-0.0045 (9)

## supplementary materials

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N2	0.0157 (10)	0.0175 (10)	0.0176 (9)	0.0015 (8)	0.0054 (9)	-0.0003 (8)
C1	0.0153 (11)	0.0153 (12)	0.0148 (11)	0.0002 (9)	0.0058 (10)	0.0002 (9)
C2	0.0158 (12)	0.0198 (12)	0.0246 (13)	0.0035 (10)	0.0029 (11)	-0.0052 (11)
C3	0.0148 (12)	0.0172 (11)	0.0147 (11)	0.0002 (9)	0.0031 (10)	0.0018 (9)
C4	0.0188 (13)	0.0194 (12)	0.0193 (11)	-0.0026 (10)	0.0015 (11)	0.0002 (10)
C5	0.0115 (12)	0.0273 (14)	0.0216 (12)	0.0004 (9)	0.0009 (10)	0.0039 (10)
C6	0.0248 (14)	0.0213 (13)	0.0234 (13)	0.0085 (11)	0.0090 (12)	0.0048 (10)
C7	0.0188 (12)	0.0135 (11)	0.0209 (12)	0.0022 (10)	0.0070 (11)	0.0018 (10)
C8	0.0149 (12)	0.0165 (12)	0.0141 (11)	-0.0005 (9)	0.0053 (10)	0.0022 (9)
C9	0.0149 (12)	0.0169 (12)	0.0151 (11)	-0.0009 (9)	0.0048 (10)	0.0013 (9)
C10	0.0173 (12)	0.0158 (11)	0.0227 (12)	-0.0020 (10)	0.0068 (10)	-0.0043 (10)
C11	0.0156 (12)	0.0210 (13)	0.0268 (13)	0.0021 (10)	0.0090 (11)	-0.0011 (10)
C12	0.0124 (11)	0.0229 (13)	0.0198 (12)	-0.0047 (9)	0.0045 (10)	0.0007 (10)
C13	0.0212 (13)	0.0171 (11)	0.0203 (12)	-0.0051 (10)	0.0068 (11)	-0.0018 (10)
C14	0.0182 (12)	0.0200 (13)	0.0172 (11)	0.0029 (10)	0.0055 (11)	-0.0018 (10)

### *Geometric parameters (Å, °)*

Br1—C12	1.894 (2)	C6—C7	1.369 (3)
N1—C2	1.307 (3)	C6—H6	0.9500
N1—C3	1.367 (3)	C7—C8	1.413 (3)
N2—C1	1.320 (3)	C7—H7	0.9500
N2—C8	1.368 (3)	C9—C10	1.393 (3)
C1—C2	1.422 (3)	C9—C14	1.400 (3)
C1—C9	1.484 (3)	C10—C11	1.385 (3)
C2—H2	0.9500	C10—H10	0.9500
C3—C8	1.411 (3)	C11—C12	1.379 (3)
C3—C4	1.414 (3)	C11—H11	0.9500
C4—C5	1.364 (3)	C12—C13	1.383 (3)
C4—H4	0.9500	C13—C14	1.378 (3)
C5—C6	1.407 (3)	C13—H13	0.9500
C5—H5	0.9500	C14—H14	0.9500
C2—N1—C3	116.11 (19)	C8—C7—H7	120.0
C1—N2—C8	116.82 (18)	N2—C8—C3	121.6 (2)
N2—C1—C2	120.8 (2)	N2—C8—C7	119.4 (2)
N2—C1—C9	118.30 (19)	C3—C8—C7	119.0 (2)
C2—C1—C9	120.9 (2)	C10—C9—C14	118.1 (2)
N1—C2—C1	123.9 (2)	C10—C9—C1	121.96 (19)
N1—C2—H2	118.0	C14—C9—C1	119.9 (2)
C1—C2—H2	118.0	C11—C10—C9	121.1 (2)
N1—C3—C8	120.74 (19)	C11—C10—H10	119.5
N1—C3—C4	119.5 (2)	C9—C10—H10	119.5
C8—C3—C4	119.7 (2)	C12—C11—C10	119.2 (2)
C5—C4—C3	119.9 (2)	C12—C11—H11	120.4
C5—C4—H4	120.0	C10—C11—H11	120.4
C3—C4—H4	120.0	C11—C12—C13	121.2 (2)
C4—C5—C6	120.5 (2)	C11—C12—Br1	119.76 (18)
C4—C5—H5	119.7	C13—C12—Br1	119.03 (17)
C6—C5—H5	119.7	C14—C13—C12	119.1 (2)

C7—C6—C5	120.7 (2)	C14—C13—H13	120.4
C7—C6—H6	119.7	C12—C13—H13	120.4
C5—C6—H6	119.7	C13—C14—C9	121.3 (2)
C6—C7—C8	120.1 (2)	C13—C14—H14	119.4
C6—C7—H7	120.0	C9—C14—H14	119.4
C8—N2—C1—C2	0.1 (3)	C4—C3—C8—C7	-0.2 (3)
C8—N2—C1—C9	179.40 (19)	C6—C7—C8—N2	-179.0 (2)
C3—N1—C2—C1	-2.1 (3)	C6—C7—C8—C3	1.2 (3)
N2—C1—C2—N1	2.2 (4)	N2—C1—C9—C10	-176.0 (2)
C9—C1—C2—N1	-177.1 (2)	C2—C1—C9—C10	3.3 (4)
C2—N1—C3—C8	0.0 (3)	N2—C1—C9—C14	3.5 (3)
C2—N1—C3—C4	-177.7 (2)	C2—C1—C9—C14	-177.2 (2)
N1—C3—C4—C5	177.3 (2)	C14—C9—C10—C11	0.4 (4)
C8—C3—C4—C5	-0.4 (3)	C1—C9—C10—C11	179.9 (2)
C3—C4—C5—C6	0.1 (4)	C9—C10—C11—C12	-0.2 (4)
C4—C5—C6—C7	0.8 (4)	C10—C11—C12—C13	-0.6 (4)
C5—C6—C7—C8	-1.5 (4)	C10—C11—C12—Br1	179.59 (19)
C1—N2—C8—C3	-2.2 (3)	C11—C12—C13—C14	1.2 (4)
C1—N2—C8—C7	178.0 (2)	Br1—C12—C13—C14	-179.02 (17)
N1—C3—C8—N2	2.2 (3)	C12—C13—C14—C9	-1.0 (4)
C4—C3—C8—N2	179.9 (2)	C10—C9—C14—C13	0.2 (4)
N1—C3—C8—C7	-177.9 (2)	C1—C9—C14—C13	-179.4 (2)

Fig. 1

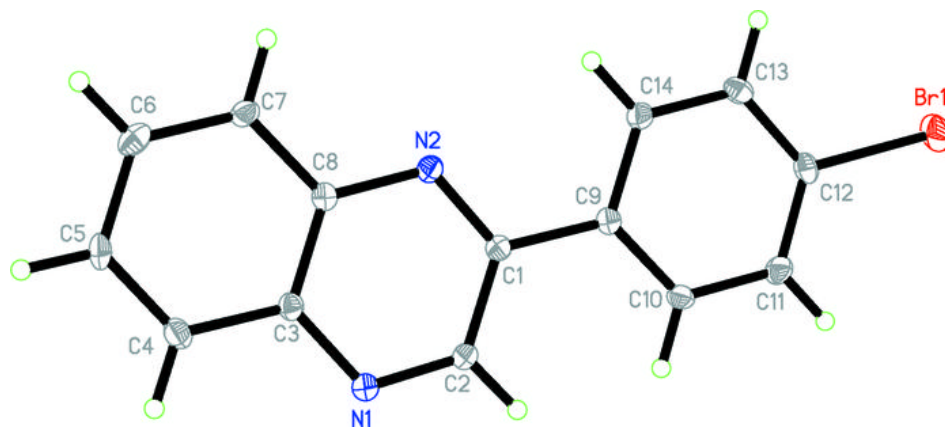




Fig. 2

