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2-(4-Bromophenyl)quinoxaline

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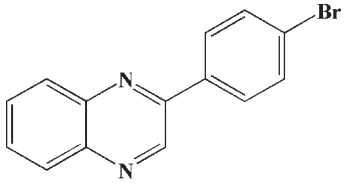
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.075; data-to-parameter ratio = 17.3.

In the title compound, $C_{14}H_9BrN_2$, 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

$C_{14}H_9BrN_2$
M_r = 285.14
Monoclinic, $P2_1/c$
a = 13.959 (3) Å
b = 5.9031 (12) Å
c = 14.497 (3) Å
β = 109.53 (3)°
V = 1125.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.63 mm^{-1}
T = 153 K
0.20 × 0.18 × 0.10 mm

Data collection

Rigaku MM-OO7/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_{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
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

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).

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supporting information

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2-(4-Bromophenyl)quinoxaline

Zhi-jian Wang, Wei-min Jia, Hong-guo Yao, Hong Qiu and Wei Wang

S1. 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 derivates 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)°, which means that the benzene ring and the quinoxaline ring are approximately coplanar with a r.m.s deviation of 0.0285 (3) Å, the Br atom lying in the plane of the substituent benzene ring [r.m.s deviation, 0.0271 (3) Å]. The crystal packing (Fig. 2) is stabilized by van der Waals forces.

S2. 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).

S3. Refinement

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

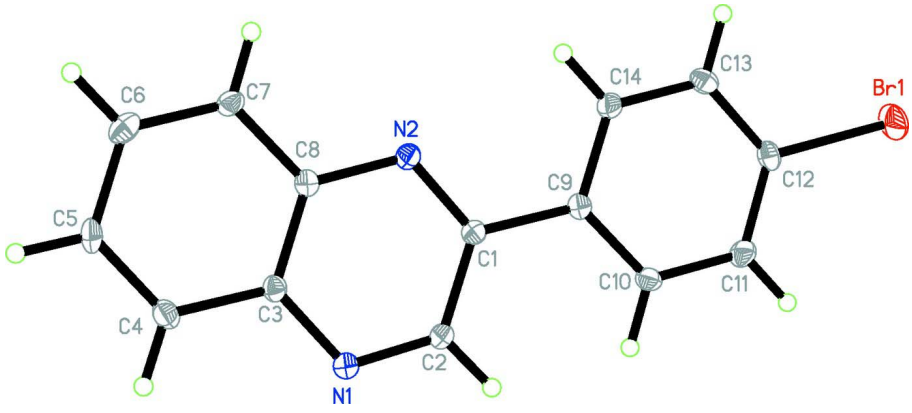

Figure 1

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

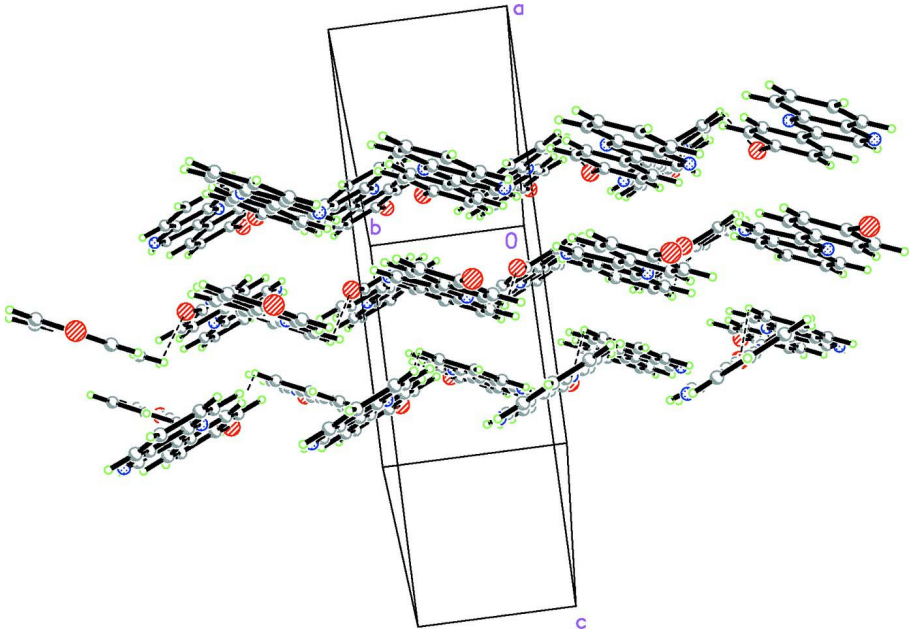

Figure 2

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

2-(4-Bromophenyl)quinoxaline

Crystal data

$C_{14}H_9BrN_2$
$M_r = 285.14$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.959\ (3)$ Å
$b = 5.9031\ (12)$ Å
$c = 14.497\ (3)$ Å
$\beta = 109.53\ (3)°$
$V = 1125.9\ (4)$ Å^3
$Z = 4$

$F(000) = 568$
$D_x = 1.682$ Mg m^{-3}
Melting point: 418 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3221 reflections
$\theta = 2.9–27.9°$
$\mu = 3.63$ mm^{-1}
$T = 153$ K
Prism, colorless
0.20 × 0.18 × 0.10 mm

Data collection

Rigaku **Model name?** CCD area-detector diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 7.31 pixels mm^{-1}
φ and ω scans
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_{int} = 0.052
θ_{max} = 27.9°, θ_{min} = 2.9°
h = −18→11
k = −7→7
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.075
S = 0.96
2683 reflections
155 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
$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
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 (Å^2)

	x	y	z	U_{iso}*/U_{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 (Å²)

	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)
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, º)

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)