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The crystal structure of 7-Bromo-2-(4-chlorophenyl)-quinoxaline, $C_{14}H_9BrClN_2$

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Abstract

$C_{14}H_9BrClN_2$, monoclinic, $P2_1/n$ (no. 14), $a = 17.1347(11)$ Å, $b = 3.8441(2)$ Å, $c = 18.4127(12)$ Å, $\beta = 97.861(2)^\circ$, $V = 1201.40(13)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0388$, $wR_{ref}(F^2) = 0.1302$, $T = 170$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

In a specific experiment, 1.86 g (10.0 mmol) 4-bromobenzene-1,2-diamine was initially dissolved in 40 mL toluene. About 1.55 g (11.0 mmol) 4-chlorobenzaldehyde was added to this

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.15 × 0.11 × 0.08 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	3.62 mm ⁻¹
Diffractometer, scan mode:	D8 VENTURE, φ and ω
θ_{max} , completeness:	26.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	12,671, 2469, 0.061
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1895
$N(param)_{refined}$:	163
Programs:	Bruker [1], SHELX [2, 3], Olex2 [4]

solution and stirred for 5 min. Then 1.95 g (10.0 mmol) tosylmethyl isocyanide and 1.35 g (12.0 mmol) triethylene diamine were added. Subsequently, the mixture was heated to 80 °C and stirred for 4 h. The resulting solution was sequentially washed with hydrochloric acid (5%) and H₂O. The organic compound was concentrated under reduced pressure and separated by silica-gel column chromatography with an ethyl acetate and petroleum ether (10%) mixture. Crystals obtained after slow evaporation of a combination of petroleum ether and ethyl acetate at room temperature within a week.

Experimental details

All hydrogen atoms were placed in calculated positions ($C-H = 0.95$ Å) and refined as riding atoms. The U_{iso} values were constrained to be $1.2U_{eq}$. All the H atoms were refined as riding on their parent atom.

Comment

Quinoxaline, also known as benzopyrazine, is a bicyclic heterocyclic molecule composed of pyrazine and benzene rings. It has three other isomers, such as quinazoline, cinolin, and *o*-benzodiazine. Quinoxaline derivatives are widely used in industry [5, 6], dyes [7–9], and antibiotics [10–12]. They are essential in the industry because they can inhibit metal corrosion [5, 6]. And they can be used in dyes and electroluminescent materials because they have chromophores similar to natural systems. Additionally, they have attracted significant attention in the

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Br1	0.37170 (2)	0.66309 (11)	0.87227 (2)	0.03856 (19)
C1	0.4771 (2)	0.5789 (10)	0.7680 (2)	0.0294 (8)
H1	0.514521	0.682332	0.804515	0.035*
C2	0.4994 (2)	0.4754 (10)	0.70059 (19)	0.0273 (8)
C3	0.4430 (2)	0.3159 (9)	0.64800 (19)	0.0267 (8)
C4	0.3647 (2)	0.2718 (10)	0.6626 (2)	0.0327 (9)
H4	0.326420	0.169797	0.626665	0.039*
C5	0.3441 (2)	0.3757 (9)	0.7283 (2)	0.0330 (9)
H5	0.291675	0.344814	0.738596	0.040*
C6	0.4015 (2)	0.5294 (10)	0.78053 (19)	0.0296 (8)
C7	0.5366 (2)	0.2501 (10)	0.5724 (2)	0.0292 (8)
H7	0.552724	0.172374	0.527811	0.035*
C8	0.5938 (2)	0.4167 (9)	0.62477 (19)	0.0251 (8)
C9	0.6756 (2)	0.4743 (10)	0.60847 (19)	0.0263 (8)
C10	0.7310 (2)	0.6244 (9)	0.6621 (2)	0.0278 (8)
H10	0.715567	0.690231	0.707804	0.033*
C11	0.8080 (2)	0.6787 (10)	0.6498 (2)	0.0308 (8)
H11	0.845049	0.784634	0.686239	0.037*
C12	0.8301 (2)	0.5763 (10)	0.5835 (2)	0.0296 (8)
C13	0.7768 (2)	0.4293 (11)	0.5296 (2)	0.0320 (9)
H13	0.792527	0.364877	0.483959	0.038*
C14	0.6996 (2)	0.3756 (9)	0.5424 (2)	0.0306 (9)
H14	0.662893	0.270396	0.505580	0.037*
Cl1	0.92654 (6)	0.6448 (3)	0.56695 (6)	0.0400 (3)
N1	0.46344 (18)	0.1985 (8)	0.58250 (17)	0.0292 (7)
N2	0.57492 (17)	0.5262 (8)	0.68817 (15)	0.0266 (7)

pharmacology industry because of their extensive biological characteristics. For example, they can fight against bacteria, fungi, viruses, Leishmania, tuberculosis, malaria, cancer, depression, and nervous activity. At present, many new compounds assembled with quinoxaline structure as precursors have been characterised [13–18].

The asymmetric unit consists of one 7-bromo-2-(4-chloro-phenyl)-quinoxaline molecule. There is a bromine substituent bearing in the benzene ring of quinoxaline molecules, and the measured length of the C–Br bond is 1.901(4) Å. There is a chlorobenzene group substituted on the pyrazine ring at the *para* position of the chlorobenzene substituent, and the measured length of the C–C bond for C8–C9 is 1.490(6) Å. The size of the C–Cl bond in the chlorobenzene substituent is 1.741(4) Å. The two benzene rings are not entirely symmetrical. In the benzene ring of quinoxaline, the angle range of C–C–C is 119.1(4)–122.4(4)° with the minimum angle on the unsubstituted carbon atom and the maximum angle on the carbon atom with bromine substituent. In the benzene ring of chlorobenzene substituent, the angle range of C–C–C is 118.5(4)–121.2(4)° with the minimum angle on the carbon atom substituted by quinoxaline and the maximum angle on the carbon atom with chlorine

substituent. C1...C6 and C9...C12 benzene rings are inclined to the average plane of heterocycles by 177.04(3)° and 176.5(3)° respectively, indicating that the styryl part is almost coplanar with the quinoxaline unit. For the given formula, all bond distances and angles are consistent with the expectation and in accord with the parent structure [19].

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