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2-(4-Fluorophenyl)quinoxaline

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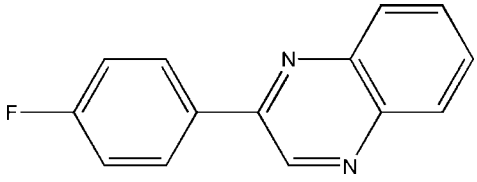
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.109; data-to-parameter ratio = 15.9.

In the title compound, $C_{14}H_9FN_2$, the dihedral angle between the benzene ring and the quinoxaline ring system is 22.2 (3)°. Any aromatic π–π stacking in the crystal must be very weak, with a minimum centroid–centroid separation of 3.995 (2) Å.

Related literature

For background to the applications of quinoxaline derivatives, see: Lindsley *et al.* (2005); Dailey *et al.* (2001).



Experimental

Crystal data

$C_{14}H_9FN_2$
M_r = 224.23
Monoclinic, $C2/c$
a = 24.249 (13) Å
b = 3.7925 (19) Å
c = 22.609 (13) Å
β = 91.866 (9)°
V = 2078.2 (19) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 113 K
0.20 × 0.18 × 0.10 mm

Data collection

Rigaku Saturn724 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
T_{min} = 0.981, T_{max} = 0.990
9711 measured reflections
2454 independent reflections
1797 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.109
S = 1.01
2454 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2008); 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: HB6725).

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supplementary materials

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Comment

Quinoxaline and its derivatives are an important class of nitrogen-containing heterocycles displaying both biologial activities (Lindsley *et al.*, 2005) and technological applications (Dailey *et al.*, 2001). Here, we report the synthesis and crystal structure of the title compound (Fig. 1).

In the title compound, $C_{14}H_9FN_2$, the dihedral angle between the benzene ring and the quinoxaline ring is 22.2 (3)°.

Experimental

A solution of benzene-1,2-diamine (1.5 mmol) and 2-(4-fluorophenyl)-2-oxoacetaldehyde monohydrate (1.5 mmol) in EtOH (10 ml) was stirred at room temperature for 0.5 h. After completion of the reaction (monitored by TLC or HPLC), the precipitated solid was collected by filtration and dried to afford the pure product. Or after completion of the reaction, water was added to the reaction mixture and filtered to afford the product. When necessary, the product was recrystallized from ethanol/water. Colourless prisms were grown by slow evaporation of a solution in chloroform/ethanol (1:1).

Refinement

H atoms were placed in calculated positions (C—H = 0.95 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Computing details

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear* (Rigaku, 2008); data reduction: *CrystalClear* (Rigaku, 2008); 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* (Sheldrick, 2008).

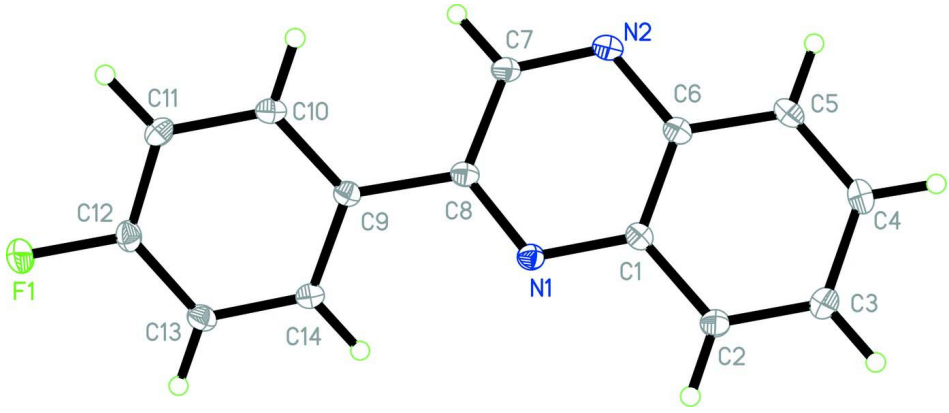

Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids for the non-hydrogen atoms.

2-(4-Fluorophenyl)quinoxaline

Crystal data

$C_{14}H_9FN_2$
$M_r = 224.23$
Monoclinic, $C2/c$
$a = 24.249\ (13)$ Å
$b = 3.7925\ (19)$ Å
$c = 22.609\ (13)$ Å
$\beta = 91.866\ (9)°$
$V = 2078.2\ (19)$ Å^3
$Z = 8$
$F(000) = 928$
$D_x = 1.433$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3509 reflections
$\theta = 1.7–27.9°$
$\mu = 0.10$ mm^{-1}
$T = 113$ K
Prism, colorless
0.20 × 0.18 × 0.10 mm

Data collection

Rigaku Saturn724 CCD diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.22 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
$T_{min} = 0.981$, $T_{max} = 0.990$
9711 measured reflections
2454 independent reflections
1797 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 27.9°$, $\theta_{min} = 1.7°$
$h = -31\rightarrow31$
$k = -4\rightarrow4$
$l = -29\rightarrow29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.109$
$S = 1.01$
2454 reflections
154 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
$w = 1/[\sigma^2(F_o^2) + (0.0692P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.46580 (3)	0.67692 (19)	1.18737 (3)	0.0321 (2)
N1	0.39311 (3)	0.1470 (2)	0.93164 (4)	0.0184 (2)
N2	0.28374 (3)	−0.1127 (2)	0.93193 (4)	0.0213 (2)
C1	0.36818 (4)	0.0119 (3)	0.88147 (4)	0.0182 (2)
C2	0.39774 (4)	−0.0011 (3)	0.82863 (5)	0.0216 (3)
H2	0.4347	0.0813	0.8283	0.026*
C3	0.37306 (5)	−0.1322 (3)	0.77801 (5)	0.0238 (3)
H3	0.3931	−0.1408	0.7426	0.029*
C4	0.31805 (5)	−0.2552 (3)	0.77785 (5)	0.0246 (3)
H4	0.3013	−0.3434	0.7423	0.030*
C5	0.28877 (4)	−0.2481 (3)	0.82842 (5)	0.0226 (3)
H5	0.2519	−0.3332	0.8280	0.027*
C6	0.31319 (4)	−0.1147 (3)	0.88123 (5)	0.0189 (2)
C7	0.30886 (4)	0.0153 (3)	0.97928 (5)	0.0205 (2)
H7	0.2895	0.0180	1.0152	0.025*
C8	0.36398 (4)	0.1514 (3)	0.97994 (5)	0.0175 (2)
C9	0.38994 (4)	0.2927 (3)	1.03511 (4)	0.0173 (2)
C10	0.35866 (4)	0.4178 (3)	1.08148 (5)	0.0204 (3)
H10	0.3195	0.4132	1.0779	0.025*
C11	0.38416 (5)	0.5485 (3)	1.13269 (5)	0.0217 (3)
H11	0.3630	0.6352	1.1642	0.026*
C12	0.44101 (5)	0.5499 (3)	1.13683 (5)	0.0217 (3)
C13	0.47352 (4)	0.4309 (3)	1.09221 (5)	0.0220 (3)
H13	0.5126	0.4356	1.0963	0.026*
C14	0.44741 (4)	0.3042 (3)	1.04120 (5)	0.0193 (2)
H14	0.4690	0.2235	1.0096	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0308 (4)	0.0440 (5)	0.0213 (4)	−0.0068 (3)	−0.0033 (3)	−0.0063 (3)
N1	0.0176 (4)	0.0186 (5)	0.0190 (4)	−0.0001 (4)	0.0009 (3)	0.0012 (4)
N2	0.0164 (4)	0.0220 (5)	0.0256 (5)	−0.0004 (4)	0.0011 (4)	0.0017 (4)
C1	0.0184 (5)	0.0157 (5)	0.0204 (5)	0.0005 (4)	−0.0014 (4)	0.0015 (4)
C2	0.0208 (5)	0.0212 (6)	0.0228 (6)	−0.0016 (4)	0.0017 (4)	0.0009 (4)
C3	0.0282 (6)	0.0227 (6)	0.0206 (5)	0.0005 (5)	0.0023 (4)	0.0004 (5)
C4	0.0279 (6)	0.0225 (6)	0.0229 (6)	0.0010 (5)	−0.0066 (4)	−0.0017 (5)

C5	0.0183 (5)	0.0208 (6)	0.0284 (6)	0.0000 (4)	−0.0045 (5)	−0.0002 (5)
C6	0.0180 (5)	0.0152 (5)	0.0233 (5)	0.0018 (4)	−0.0011 (4)	0.0023 (4)
C7	0.0164 (5)	0.0225 (6)	0.0226 (5)	−0.0002 (4)	0.0021 (4)	0.0026 (4)
C8	0.0156 (5)	0.0161 (6)	0.0207 (5)	0.0020 (4)	0.0002 (4)	0.0031 (4)
C9	0.0177 (5)	0.0159 (5)	0.0182 (5)	−0.0010 (4)	0.0007 (4)	0.0034 (4)
C10	0.0163 (5)	0.0224 (6)	0.0227 (5)	0.0008 (4)	0.0022 (4)	0.0032 (4)
C11	0.0245 (5)	0.0228 (6)	0.0183 (5)	0.0011 (5)	0.0050 (4)	0.0013 (4)
C12	0.0260 (5)	0.0221 (6)	0.0169 (5)	−0.0035 (4)	−0.0024 (4)	0.0007 (4)
C13	0.0176 (5)	0.0247 (6)	0.0235 (5)	−0.0008 (4)	−0.0010 (4)	0.0018 (5)
C14	0.0176 (5)	0.0196 (6)	0.0208 (5)	0.0007 (4)	0.0027 (4)	0.0012 (4)

Geometric parameters (Å, º)

F1—C12	1.3617 (13)	C5—H5	0.9500
N1—C8	1.3198 (14)	C7—C8	1.4325 (15)
N1—C1	1.3676 (14)	C7—H7	0.9500
N2—C7	1.3078 (15)	C8—C9	1.4792 (16)
N2—C6	1.3703 (14)	C9—C14	1.3966 (15)
C1—C2	1.4138 (16)	C9—C10	1.3969 (15)
C1—C6	1.4171 (16)	C10—C11	1.3864 (16)
C2—C3	1.3676 (16)	C10—H10	0.9500
C2—H2	0.9500	C11—C12	1.3787 (17)
C3—C4	1.4131 (17)	C11—H11	0.9500
C3—H3	0.9500	C12—C13	1.3764 (16)
C4—C5	1.3656 (16)	C13—C14	1.3835 (15)
C4—H4	0.9500	C13—H13	0.9500
C5—C6	1.4095 (16)	C14—H14	0.9500
C8—N1—C1	117.21 (9)	C8—C7—H7	118.3
C7—N2—C6	116.44 (10)	N1—C8—C7	120.74 (10)
N1—C1—C2	119.44 (10)	N1—C8—C9	118.54 (10)
N1—C1—C6	121.36 (10)	C7—C8—C9	120.71 (9)
C2—C1—C6	119.20 (10)	C14—C9—C10	118.67 (10)
C3—C2—C1	119.98 (11)	C14—C9—C8	119.37 (9)
C3—C2—H2	120.0	C10—C9—C8	121.96 (10)
C1—C2—H2	120.0	C11—C10—C9	120.66 (10)
C2—C3—C4	120.63 (10)	C11—C10—H10	119.7
C2—C3—H3	119.7	C9—C10—H10	119.7
C4—C3—H3	119.7	C12—C11—C10	118.41 (10)
C5—C4—C3	120.52 (10)	C12—C11—H11	120.8
C5—C4—H4	119.7	C10—C11—H11	120.8
C3—C4—H4	119.7	F1—C12—C13	118.89 (10)
C4—C5—C6	120.05 (10)	F1—C12—C11	118.13 (10)
C4—C5—H5	120.0	C13—C12—C11	122.98 (10)
C6—C5—H5	120.0	C12—C13—C14	117.86 (10)
N2—C6—C5	119.65 (10)	C12—C13—H13	121.1
N2—C6—C1	120.73 (10)	C14—C13—H13	121.1
C5—C6—C1	119.61 (10)	C13—C14—C9	121.40 (10)
N2—C7—C8	123.50 (10)	C13—C14—H14	119.3
N2—C7—H7	118.3	C9—C14—H14	119.3

C8—N1—C1—C2	−179.57 (9)	C1—N1—C8—C9	179.40 (9)
C8—N1—C1—C6	0.65 (15)	N2—C7—C8—N1	−1.44 (17)
N1—C1—C2—C3	−179.32 (10)	N2—C7—C8—C9	179.95 (10)
C6—C1—C2—C3	0.47 (16)	N1—C8—C9—C14	−21.66 (15)
C1—C2—C3—C4	0.10 (17)	C7—C8—C9—C14	156.99 (10)
C2—C3—C4—C5	−0.63 (17)	N1—C8—C9—C10	157.91 (10)
C3—C4—C5—C6	0.56 (17)	C7—C8—C9—C10	−23.44 (16)
C7—N2—C6—C5	−179.90 (10)	C14—C9—C10—C11	−0.46 (16)
C7—N2—C6—C1	0.90 (15)	C8—C9—C10—C11	179.97 (10)
C4—C5—C6—N2	−179.19 (10)	C9—C10—C11—C12	−0.40 (16)
C4—C5—C6—C1	0.02 (16)	C10—C11—C12—F1	−179.66 (10)
N1—C1—C6—N2	−1.55 (16)	C10—C11—C12—C13	0.72 (17)
C2—C1—C6—N2	178.67 (9)	F1—C12—C13—C14	−179.76 (9)
N1—C1—C6—C5	179.25 (9)	C11—C12—C13—C14	−0.15 (18)
C2—C1—C6—C5	−0.53 (15)	C12—C13—C14—C9	−0.76 (16)
C6—N2—C7—C8	0.53 (16)	C10—C9—C14—C13	1.06 (16)
C1—N1—C8—C7	0.76 (15)	C8—C9—C14—C13	−179.36 (9)