Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Chloroquinoxaline

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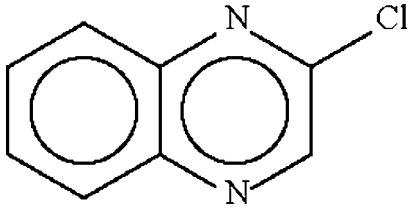
Received 29 January 2009; accepted 29 January 2009

Key indicators: single-crystal X-ray study; T = 118 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.099; data-to-parameter ratio = 16.6.

In the title compound, $C_8H_5ClN_2$, the planar molecules are arranged with their Cl atoms in close contact [Cl···Cl = 3.808 (1) and 3.881 (1) Å], indicating weak Cl···Cl interactions, which give rise to a supramolecular chain.

Related literature

The title compound is a reagent in the synthesis of chloroquinoxaline sulfamide, which is active against human cancers. For the synthesis of other phamaceutically active derivatives through conventional and other synthetic routes, see: Bhattacharjee *et al.* (2008); Cuenca *et al.* (2008); Hassan *et al.* (2006); Rangisetty *et al.* (2001); Rizzo *et al.* (2002); Sugimoto *et al.* (2003).



Experimental

Crystal data

$C_8H_5ClN_2$ M_r = 164.59
Monoclinic, $P2_1/n$
a = 9.1299 (2) Å
b = 3.8082 (1) Å
c = 21.0777 (6) Å
β = 93.028 (2)°
V = 731.82 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.44 mm^{-1}
T = 118 (2) K
0.20 × 0.06 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.916, T_{max} = 0.991
6145 measured reflections
1659 independent reflections
1173 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.099
S = 1.03
1659 reflections
100 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

I thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2366).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bhattacharjee, G., Sondhi, S. M., Dinodia, M. & Mishra, S. K. (2008). *Ind. J. Chem. Technol.* **15**, 72–74.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cuenca, A., Perez, S., Yepez, A., Paredes, L., Montecinos, L., Llovera, L. & Rodriguez, C. (2008). *J. Heterocycl. Chem.* **45**, 1199–1201.
Hassan, S. Y., Khattab, S. N., Bekhit, A. A. & Amer, A. (2006). *Bioorg. Med. Chem. Lett.* **16**, 1753–1756.
Rangisetty, J. B., Gupta, C. N. V. H. B., Prasad, A. L., Srinivas, P., Sridhar, N., Parimoo, P. & Veeranjaneyulu, A. (2001). *J. Pharm. Pharmacol.* **53**, 1409–1413.
Rizzo, A., Campos, G., Alvarez, A. & Cuenca, A. (2002). *Synth. Commun.* **32**, 813–817.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sugimoto, O., Yamada, S. & Tanji, K. (2003). *J. Org. Chem.* **68**, 2054–2057.
Westrip, S. P. (2009). *publCIF*. In preparation.

supporting information

Acta Cryst. (2009). E**65**, o455 [doi:10.1107/S1600536809003717]

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S1. Experimental

The compound was returned unchanged in an attempt at coupling it wih benzoquinone. Crystals were obtained from recrystallization from a chloroform/ether mixture.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C).

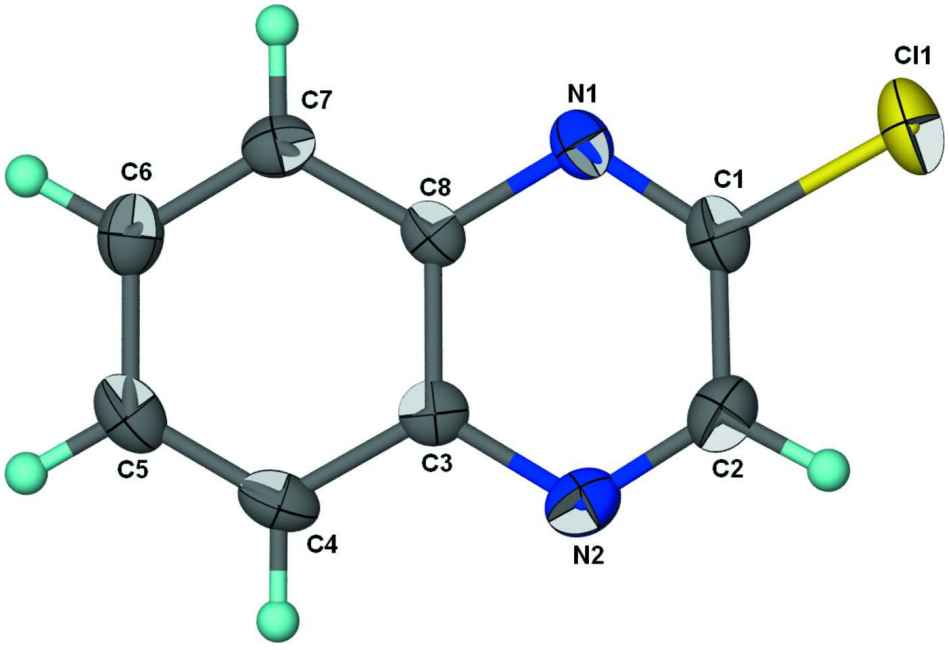

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_8H_5ClN_2$; ellipsoids are drawn at the 70% probability level and H atoms of arbitrary radius.

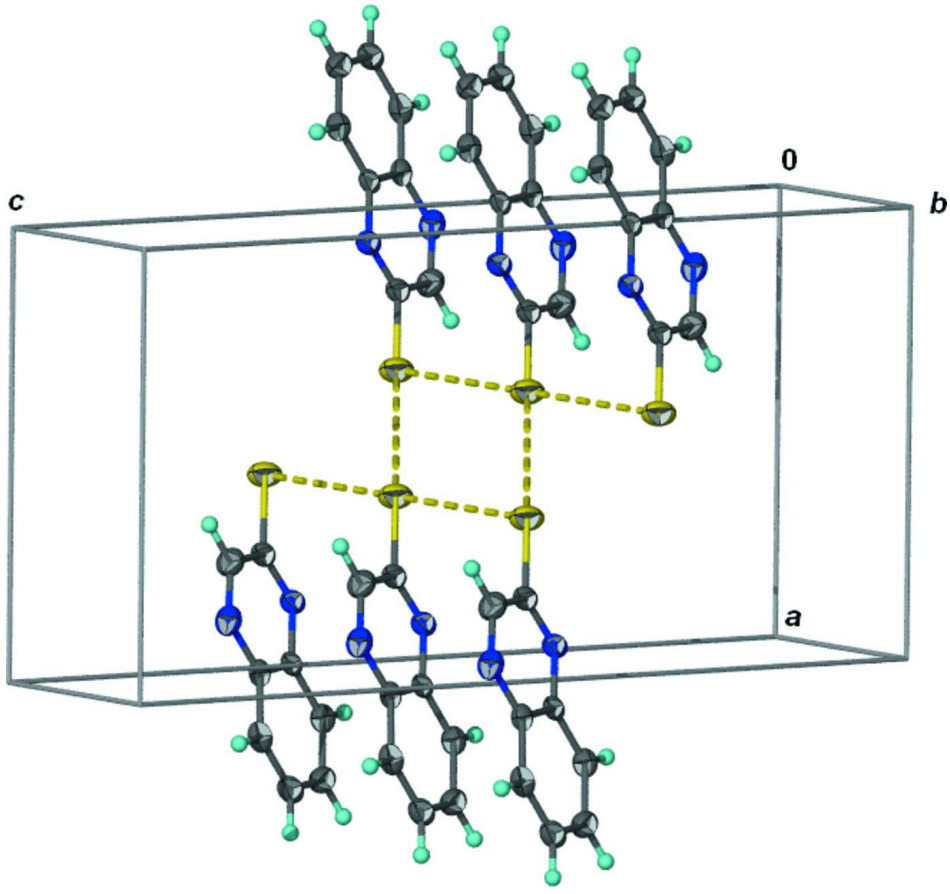

Figure 2

Chain structure in $C_8H_5ClN_2$; the Cl···Cl contacts are shown as dashed bonds.

2-Chloroquinoxaline

Crystal data

$C_8H_5ClN_2$
$M_r = 164.59$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.1299$ (2) Å
$b = 3.8082$ (1) Å
$c = 21.0777$ (6) Å
$\beta = 93.028$ (2)°
$V = 731.82$ (3) Å^3
$Z = 4$

$F(000) = 336$
$D_x = 1.494$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1328 reflections
$\theta = 2.4$–$28.1°$
$\mu = 0.44$ mm^{-1}
$T = 118$ K
Prism, colorless
0.20 × 0.06 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.916$, $T_{max} = 0.991$

6145 measured reflections
1659 independent reflections
1173 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.9°$
$h = -11 \rightarrow 11$
$k = -4 \rightarrow 4$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.099$
$S = 1.03$
1659 reflections
100 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
$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 0.1632P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.60849 (6)	0.47749 (15)	0.58158 (3)	0.03308 (19)
N1	0.88157 (18)	0.6668 (4)	0.57567 (8)	0.0202 (4)
N2	0.8977 (2)	0.9189 (4)	0.70202 (8)	0.0248 (4)
C1	0.7733 (2)	0.6552 (5)	0.61274 (10)	0.0219 (5)
C2	0.7783 (2)	0.7779 (6)	0.67617 (10)	0.0261 (5)
H2	0.6938	0.7575	0.7003	0.031*
C3	1.0163 (2)	0.9407 (5)	0.66453 (9)	0.0194 (4)
C4	1.1478 (2)	1.0934 (5)	0.68919 (10)	0.0231 (5)
H4	1.1540	1.1816	0.7314	0.028*
C5	1.2662 (2)	1.1150 (5)	0.65264 (10)	0.0250 (5)
H5	1.3549	1.2165	0.6696	0.030*
C6	1.2576 (2)	0.9872 (5)	0.58970 (10)	0.0254 (5)
H6	1.3408	1.0049	0.5646	0.030*
C7	1.1318 (2)	0.8385 (5)	0.56422 (10)	0.0214 (4)
H7	1.1275	0.7528	0.5218	0.026*
C8	1.0086 (2)	0.8132 (5)	0.60139 (9)	0.0179 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0215 (3)	0.0305 (3)	0.0466 (4)	−0.0056 (2)	−0.0042 (2)	0.0009 (3)
N1	0.0187 (9)	0.0178 (8)	0.0239 (9)	0.0000 (7)	−0.0020 (7)	0.0008 (7)
N2	0.0286 (10)	0.0243 (9)	0.0219 (9)	0.0009 (8)	0.0049 (8)	0.0013 (7)
C1	0.0190 (10)	0.0185 (10)	0.0277 (11)	−0.0005 (8)	−0.0029 (9)	0.0043 (9)
C2	0.0252 (12)	0.0257 (11)	0.0278 (12)	0.0006 (9)	0.0067 (9)	0.0018 (10)
C3	0.0234 (10)	0.0148 (9)	0.0200 (10)	0.0022 (8)	0.0005 (8)	0.0027 (8)
C4	0.0316 (12)	0.0177 (10)	0.0194 (11)	−0.0007 (8)	−0.0047 (9)	−0.0008 (8)
C5	0.0247 (11)	0.0198 (10)	0.0296 (12)	−0.0018 (8)	−0.0066 (9)	0.0028 (9)
C6	0.0222 (11)	0.0232 (11)	0.0310 (12)	−0.0007 (9)	0.0032 (9)	0.0045 (10)
C7	0.0256 (11)	0.0192 (10)	0.0195 (10)	0.0028 (9)	0.0019 (8)	0.0000 (9)
C8	0.0188 (10)	0.0144 (9)	0.0201 (10)	0.0014 (8)	−0.0031 (8)	0.0028 (8)

Geometric parameters (Å, º)

Cl1—C1	1.746 (2)	C4—C5	1.363 (3)
N1—C1	1.293 (3)	C4—H4	0.9500
N1—C8	1.372 (2)	C5—C6	1.411 (3)
N2—C2	1.308 (3)	C5—H5	0.9500
N2—C3	1.376 (3)	C6—C7	1.365 (3)
C1—C2	1.415 (3)	C6—H6	0.9500
C2—H2	0.9500	C7—C8	1.408 (3)
C3—C4	1.409 (3)	C7—H7	0.9500
C3—C8	1.415 (3)		
C1—N1—C8	115.61 (17)	C3—C4—H4	119.9
C2—N2—C3	116.68 (18)	C4—C5—C6	120.3 (2)
N1—C1—C2	124.93 (19)	C4—C5—H5	119.9
N1—C1—Cl1	117.21 (16)	C6—C5—H5	119.9
C2—C1—Cl1	117.87 (16)	C7—C6—C5	121.13 (19)
N2—C2—C1	120.92 (19)	C7—C6—H6	119.4
N2—C2—H2	119.5	C5—C6—H6	119.4
C1—C2—H2	119.5	C6—C7—C8	119.33 (19)
N2—C3—C4	119.62 (18)	C6—C7—H7	120.3
N2—C3—C8	121.21 (18)	C8—C7—H7	120.3
C4—C3—C8	119.18 (18)	N1—C8—C7	119.43 (18)
C5—C4—C3	120.18 (19)	N1—C8—C3	120.65 (18)
C5—C4—H4	119.9	C7—C8—C3	119.91 (18)
C8—N1—C1—C2	−0.5 (3)	C4—C5—C6—C7	−0.3 (3)
C8—N1—C1—Cl1	178.97 (14)	C5—C6—C7—C8	0.2 (3)
C3—N2—C2—C1	0.0 (3)	C1—N1—C8—C7	−179.61 (18)
N1—C1—C2—N2	0.6 (3)	C1—N1—C8—C3	0.0 (3)
Cl1—C1—C2—N2	−178.91 (16)	C6—C7—C8—N1	179.40 (18)
C2—N2—C3—C4	179.27 (19)	C6—C7—C8—C3	−0.2 (3)
C2—N2—C3—C8	−0.5 (3)	N2—C3—C8—N1	0.6 (3)
N2—C3—C4—C5	179.69 (18)	C4—C3—C8—N1	−179.22 (18)
C8—C3—C4—C5	−0.5 (3)	N2—C3—C8—C7	−179.87 (17)
C3—C4—C5—C6	0.5 (3)	C4—C3—C8—C7	0.3 (3)