IUCrData

ISSN 2414-3146

6,7-Dichloro-2-methyl-3-phenylquinoxaline

Myron W. Jones,[a] Katelyn M. Aldridge[b] and Guy Crundwell[b]*

[a]Department of Chemistry, Southern Illinois University Edwardsville, Edwardsville, IL 62026-1652, USA, and [b]Department of Chemistry & Biochemistry, Central Connecticut State University, 1619 Stanley Street, New Britain, CT 06053, USA. *Correspondence e-mail: crundwellg@ccsu.edu

Received 20 August 2026
Accepted 27 August 2026

Edited by M. Zeller, Purdue University, USA

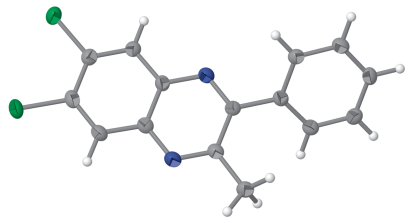
Keywords: crystal structure; quinoxaline.

CCDC reference: 2583897

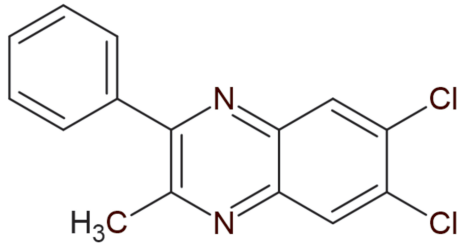
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{15}H_{10}Cl_2N_2$, was synthesized using the acid catalyst NH_4HF_2 in a water/methanol solution. The dihedral angle between the phenyl ring and the quinoxaline unit is 39.80 (5)°. There is an intermolecular hydrogen-bonding-like interaction with a neighboring chlorine atom at a distance of 2.76 Å. The extended structure features offset-stacked quinoxaline units along the [100] direction.

3D view



Chemical scheme



Structure description

In general, quinoxalines are of interest as potential antibacterial (Parhi *et al.*, 2013), antimicrobial (Singh *et al.*, 2010), and antifungal medicines (Tang *et al.*, 2022) and therefore exploring their synthesis and structures are of interest. The title compound was synthesized via a condensation reaction of a diamine and diketone using a water/methanol solution containing the NH_4HF_2 catalyst (Lassagne *et al.*, 2015).

The molecular structure is shown in Fig. 1. The quinoxaline ring system is essentially planar. The r.m.s. deviation of the dichloroquinoxaline unit (using atoms C1–C9, N1, N2, Cl1, and Cl2) is only 0.0604 Å. The quinoxaline moiety makes an angle of 39.80 (5)° with respect to the phenyl ring. There is a hydrogen-bonding-like interaction between a carbon hydrogen and a neighboring chlorine atom (Table 1). Molecules stack along the [100] direction of the unit cell (Fig. 2). Analysis of ring interactions using *PLATON* (Spek, 2009) indicats that the quinoxaline ring system (C1–C6,C8,C9,N1,N2) exhibits $\pi\cdots\pi$ stacking with interplanar spacings of 3.5039 (7) Å [for neighbor at $(1-x, -y, z)$], 3.4022 (7) Å [for neighbor at $(\frac{3}{2}-x, y, -\frac{1}{2}+z)$], and 3.3845 (7) Å [for neighbor at $(\frac{3}{2}-x, y, 1/2+z)$] with slippages of 1.515, 3.582, and 3.565Å, respectively..

Synthesis and crystallization

In a 50 mL Erlenmeyer flask, 1.49 g of 1-phenyl-1,2-propanedione (10.0 mmol) were added to 2 mL of H_2O and 20 mL of a 2.5 x 10^{-3} *M* methanol solution of NH_4HF_2

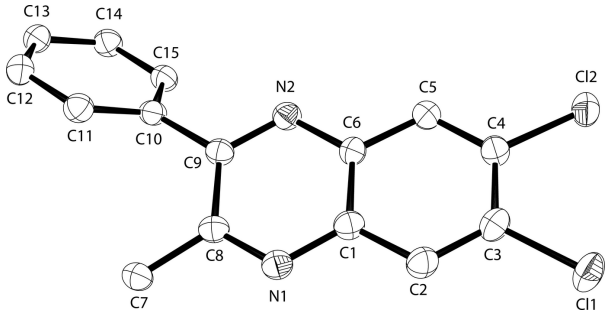


Figure 1
A view of the title molecule. Hydrogen atoms are omitted and displacement ellipsoids are drawn at the 50% probability level.

(Lassagne *et al.*, 2015). To this mixture 1.78 g of 4,5-dichloro-1,2-phenylenediamine (10.0 mmol) were added. The solution was stirred for 24 h during which the product precipitated as a pale light-tan product. 2.65 g of crude product were isolated and recrysallized from methanol solution yielding 1.92 g of purified product (66%). Crystals for the diffraction study were isolated by the slow evaporation of 50/50 hexane/ethyl acetate solutions. M.p: 426 K; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 2.78 (*s*, 3H), 7.55 (*m*, 3H), 7.64 (*m*, 2H), 8.17 (*s*, 1H), 8.22 (*s*, 1H); ^{13}C NMR ($CDCl_3$, 300 MHz): δ = 24.51, 128.85, 128.91, 129.16, 129.43, 129.84, 133.65, 134.12, 138.31, 139.77, 139.86, 153.98, 155.89.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

This work was supported by a CCSU-AAUP grant. All data were collected at Purdue University by Dr Matthias Zeller as part of the American Crystallographic Association Summer Course (2026). Dr Zeller also assisted with the refinement.

References

Bruker (2026). *APEX6* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

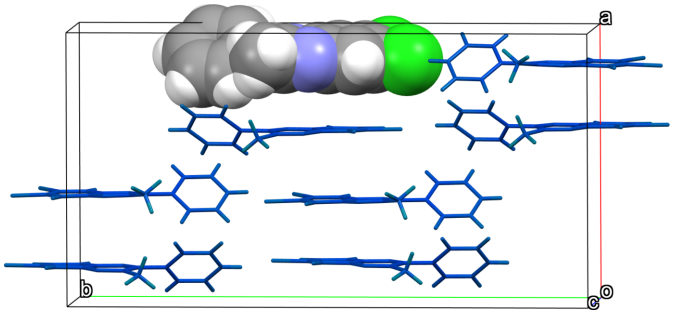


Figure 2
A view of the unit-cell packing along the [100] direction.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Cl2^{i}	0.95	2.76	3.704 (3)	175

Symmetry code: (i) $x, y, z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{10}Cl_2N_2$
M_r	289.15
Crystal system, space group	Orthorhombic, *Aea*2
Temperature (K)	150
a, *b*, *c* (Å)	13.7569 (4), 26.2508 (8), 7.1470 (2)
V (Å^3)	2580.99 (13)
Z	8
Radiation type	Cu *K*α
μ (mm^{-1})	4.40
Crystal size (mm)	0.21 × 0.11 × 0.06
Data collection	
Diffractometer	Bruker AXS D8 Quest
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.500, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	35150, 2788, 2646
R_{int}	0.064
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.640
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.078, 1.11
No. of reflections	2788
No. of parameters	173
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.28
Absolute structure	Flack *x* determined using 1146 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.004 (7)

Computer programs: *APEX6* and *SAINT* (Bruker, 2026), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2025/1* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2020).

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Lassagne, F., Chevallier, F., Roisnel, T., Dorcet, V. & Mongin, F. (2015). *J. Synth. Org. Chem.* **47**, 2680–2689.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
Parhi, A. K., Zhang, Y., Saionz, K. W., Pradhan, P., Kaul, M., Trivedi, K., Pilch, D. S. & LaVoie, E. J. (2013). *Bioorg. Med. Chem. Lett.* **23**, 4968–4974.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Singh, D. P., Deivedi, S. K., Hashim, S. R. & Singhal, R. G. (2010). *Pharmaceuticals* **3**, 2416–2425.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Tang, X., Zhou, G., Zhan, W., Hu, D., Zhou, R., Sun, N., Chen, S., Wu, W. & Xue, W. (2022). *RCS Adv.* **12**, 2399–2407.

full crystallographic data

IUCrData (2026). **11**, x260892 [https://doi.org/10.1107/S2414314626008928]

6,7-Dichloro-2-methyl-3-phenylquinoxaline

Myron W. Jones, Katelyn M. Aldridge and Guy Crundwell

6,7-Dichloro-2-methyl-3-phenylquinoxaline

Crystal data

$C_{15}H_{10}Cl_2N_2$
M_r = 289.15
Orthorhombic, *Aea*2
a = 13.7569 (4) Å
b = 26.2508 (8) Å
c = 7.1470 (2) Å
V = 2580.99 (13) Å^3
Z = 8
F(000) = 1184
D_x = 1.488 Mg m^{-3}
Melting point: 426 K
Cu *Kα* radiation, λ = 1.54178 Å
Cell parameters from 9889 reflections
θ = 3.4–80.1°
μ = 4.40 mm^{-1}
T = 150 K
Plate, clear colourless
0.21 × 0.11 × 0.06 mm

Data collection

Bruker AXS D8 Quest diffractometer
Radiation source: I-mu-S 3.0 microsource X-ray tube
HELIOS multilayer Montel optics monochromator
Detector resolution: 7.4074 pixels mm^{-1}
ω and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.500, T_{max} = 0.754
35150 measured reflections
2788 independent reflections
2646 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 80.6°, θ_{min} = 3.4°
h = −17→17
k = −33→33
l = −8→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.078
S = 1.11
2788 reflections
173 parameters
1 restraint
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.4866P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack *x* determined using 1146 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.004 (7)

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. Hydrogen atoms on sp^2 and sp^3 carbons were placed at calculated positions with a C-H distance of 0.95 Å and 0.98 Å and were included in the refinement in riding motion approximation with $U_{iso} = 1.2U_{eq}$ or $1.5U_{eq}$ of the carrier atom, respectively.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.37186 (15)	0.47901 (10)	0.6000 (4)	0.0262 (5)
C3	0.37034 (16)	0.56404 (10)	0.4771 (4)	0.0284 (5)
C10	0.37433 (14)	0.32221 (9)	0.4945 (4)	0.0242 (5)
C15	0.42966 (17)	0.30390 (9)	0.3437 (3)	0.0258 (5)
H15	0.466810	0.327048	0.270755	0.031*
N1	0.37599 (15)	0.44750 (9)	0.7518 (3)	0.0280 (5)
Cl1	0.36731 (4)	0.62940 (2)	0.51359 (11)	0.03628 (18)
C13	0.37601 (17)	0.21837 (10)	0.4054 (4)	0.0303 (5)
H13	0.377408	0.183049	0.376637	0.036*
C6	0.37267 (16)	0.45912 (9)	0.4161 (4)	0.0242 (5)
C12	0.31946 (17)	0.23595 (9)	0.5524 (3)	0.0306 (5)
H12	0.281249	0.212716	0.622943	0.037*
Cl2	0.37977 (5)	0.58627 (2)	0.10644 (10)	0.03599 (18)
C4	0.37379 (16)	0.54433 (10)	0.2935 (4)	0.0275 (5)
C5	0.37397 (16)	0.49310 (10)	0.2613 (4)	0.0267 (5)
H5	0.374956	0.480307	0.136961	0.032*
C8	0.37819 (16)	0.39822 (10)	0.7220 (4)	0.0250 (5)
C14	0.43071 (17)	0.25251 (10)	0.3002 (4)	0.0291 (5)
H14	0.468808	0.240553	0.198416	0.035*
N2	0.37302 (13)	0.40786 (8)	0.3852 (3)	0.0259 (5)
C2	0.36965 (16)	0.53235 (11)	0.6280 (4)	0.0294 (5)
H2	0.367700	0.545967	0.751059	0.035*
C9	0.37394 (14)	0.37773 (10)	0.5335 (4)	0.0232 (5)
C11	0.31853 (16)	0.28751 (8)	0.5968 (4)	0.0276 (4)
H11	0.279563	0.299277	0.697663	0.033*
C7	0.38880 (19)	0.36530 (10)	0.8927 (4)	0.0299 (5)
H7A	0.325163	0.351482	0.927622	0.045*
H7B	0.414578	0.385727	0.996143	0.045*
H7C	0.433567	0.337216	0.865550	0.045*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0260 (11)	0.0266 (13)	0.0260 (11)	0.0011 (8)	0.0006 (10)	−0.0021 (11)
C3	0.0277 (11)	0.0226 (13)	0.0350 (14)	−0.0003 (8)	0.0032 (9)	−0.0036 (10)
C10	0.0257 (10)	0.0242 (11)	0.0228 (12)	0.0017 (7)	−0.0034 (8)	−0.0012 (10)

C15	0.0287 (10)	0.0266 (11)	0.0221 (10)	0.0002 (9)	−0.0007 (8)	0.0006 (8)
N1	0.0320 (10)	0.0285 (11)	0.0235 (10)	0.0005 (8)	0.0006 (7)	−0.0029 (9)
Cl1	0.0454 (3)	0.0214 (3)	0.0421 (4)	−0.0014 (2)	0.0073 (3)	−0.0051 (2)
C13	0.0405 (13)	0.0215 (13)	0.0289 (13)	0.0001 (9)	−0.0036 (11)	−0.0014 (10)
C6	0.0256 (11)	0.0218 (12)	0.0252 (11)	0.0012 (8)	−0.0003 (8)	−0.0007 (10)
C12	0.0354 (12)	0.0287 (12)	0.0278 (13)	−0.0049 (9)	0.0008 (8)	0.0018 (8)
Cl2	0.0506 (3)	0.0257 (3)	0.0316 (3)	−0.0025 (2)	−0.0014 (3)	0.0041 (2)
C4	0.0281 (11)	0.0266 (13)	0.0278 (13)	−0.0002 (9)	−0.0006 (9)	0.0014 (10)
C5	0.0303 (12)	0.0256 (12)	0.0241 (13)	−0.0006 (9)	−0.0005 (8)	0.0000 (10)
C8	0.0249 (11)	0.0268 (12)	0.0234 (12)	0.0001 (8)	0.0003 (8)	−0.0026 (10)
C14	0.0332 (11)	0.0294 (11)	0.0246 (10)	0.0028 (10)	0.0008 (9)	−0.0028 (9)
N2	0.0281 (10)	0.0256 (12)	0.0240 (11)	0.0018 (7)	−0.0002 (8)	−0.0016 (8)
C2	0.0346 (12)	0.0270 (13)	0.0267 (14)	0.0006 (8)	0.0027 (9)	−0.0056 (10)
C9	0.0225 (9)	0.0252 (12)	0.0220 (11)	0.0005 (7)	0.0005 (8)	0.0001 (9)
C11	0.0292 (10)	0.0281 (11)	0.0257 (10)	0.0000 (8)	0.0019 (9)	−0.0018 (9)
C7	0.0374 (12)	0.0296 (14)	0.0226 (12)	0.0005 (10)	−0.0029 (10)	−0.0008 (10)

Geometric parameters (Å, º)

C1—N1	1.365 (4)	C6—N2	1.364 (3)
C1—C6	1.415 (4)	C12—H12	0.9500
C1—C2	1.415 (4)	C12—C11	1.390 (3)
C3—Cl1	1.736 (3)	Cl2—C4	1.734 (3)
C3—C4	1.411 (4)	C4—C5	1.364 (4)
C3—C2	1.362 (4)	C5—H5	0.9500
C10—C15	1.404 (3)	C8—C9	1.451 (4)
C10—C9	1.484 (3)	C8—C7	1.502 (4)
C10—C11	1.397 (3)	C14—H14	0.9500
C15—H15	0.9500	N2—C9	1.323 (4)
C15—C14	1.385 (3)	C2—H2	0.9500
N1—C8	1.311 (3)	C11—H11	0.9500
C13—H13	0.9500	C7—H7A	0.9800
C13—C12	1.386 (4)	C7—H7B	0.9800
C13—C14	1.391 (4)	C7—H7C	0.9800
C6—C5	1.421 (3)		
N1—C1—C6	121.0 (2)	C6—C5—H5	120.4
N1—C1—C2	119.2 (3)	C4—C5—C6	119.2 (2)
C6—C1—C2	119.8 (3)	C4—C5—H5	120.4
C4—C3—Cl1	120.2 (2)	N1—C8—C9	121.0 (2)
C2—C3—Cl1	119.0 (2)	N1—C8—C7	116.0 (2)
C2—C3—C4	120.8 (2)	C9—C8—C7	123.0 (2)
C15—C10—C9	118.8 (2)	C15—C14—C13	120.0 (2)
C11—C10—C15	118.4 (2)	C15—C14—H14	120.0
C11—C10—C9	122.7 (2)	C13—C14—H14	120.0
C10—C15—H15	119.6	C9—N2—C6	117.4 (2)
C14—C15—C10	120.8 (2)	C1—C2—H2	120.2
C14—C15—H15	119.6	C3—C2—C1	119.5 (2)

C8—N1—C1	118.0 (2)	C3—C2—H2	120.2
C12—C13—H13	120.0	C8—C9—C10	122.6 (2)
C12—C13—C14	119.9 (2)	N2—C9—C10	115.9 (2)
C14—C13—H13	120.0	N2—C9—C8	121.5 (2)
C1—C6—C5	119.5 (2)	C10—C11—H11	119.7
N2—C6—C1	121.0 (2)	C12—C11—C10	120.7 (2)
N2—C6—C5	119.6 (2)	C12—C11—H11	119.7
C13—C12—H12	119.9	C8—C7—H7A	109.5
C13—C12—C11	120.1 (2)	C8—C7—H7B	109.5
C11—C12—H12	119.9	C8—C7—H7C	109.5
C3—C4—Cl2	119.1 (2)	H7A—C7—H7B	109.5
C5—C4—C3	121.2 (2)	H7A—C7—H7C	109.5
C5—C4—Cl2	119.7 (2)	H7B—C7—H7C	109.5

C1—N1—C8—C9	−1.5 (3)	C6—N2—C9—C10	−179.98 (18)
C1—N1—C8—C7	176.4 (2)	C6—N2—C9—C8	−2.3 (3)
C1—C6—C5—C4	−0.4 (3)	C12—C13—C14—C15	0.8 (4)
C1—C6—N2—C9	−0.9 (3)	Cl2—C4—C5—C6	177.70 (17)
C3—C4—C5—C6	−1.3 (3)	C4—C3—C2—C1	−0.4 (4)
C10—C15—C14—C13	0.5 (3)	C5—C6—N2—C9	178.54 (19)
C15—C10—C9—C8	−139.0 (2)	C14—C13—C12—C11	−1.1 (4)
C15—C10—C9—N2	38.6 (3)	N2—C6—C5—C4	−179.9 (2)
C15—C10—C11—C12	1.3 (3)	C2—C1—N1—C8	−179.85 (19)
N1—C1—C6—C5	−176.4 (2)	C2—C1—C6—C5	1.7 (3)
N1—C1—C6—N2	3.1 (3)	C2—C1—C6—N2	−178.80 (19)
N1—C1—C2—C3	176.8 (2)	C2—C3—C4—Cl2	−177.28 (18)
N1—C8—C9—C10	−178.79 (18)	C2—C3—C4—C5	1.7 (4)
N1—C8—C9—N2	3.7 (3)	C9—C10—C15—C14	−178.8 (2)
Cl1—C3—C4—Cl2	2.5 (3)	C9—C10—C11—C12	178.5 (2)
Cl1—C3—C4—C5	−178.48 (17)	C11—C10—C15—C14	−1.5 (3)
Cl1—C3—C2—C1	179.85 (16)	C11—C10—C9—C8	43.8 (3)
C13—C12—C11—C10	0.0 (4)	C11—C10—C9—N2	−138.6 (2)
C6—C1—N1—C8	−1.7 (3)	C7—C8—C9—C10	3.4 (3)
C6—C1—C2—C3	−1.3 (3)	C7—C8—C9—N2	−174.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cl2^{i}	0.95	2.76	3.704 (3)	175

Symmetry code: (i) *x*, *y*, *z*+1.