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2,3-Bis(4-chlorophenyl)quinoxaline

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.139
Data-to-parameter ratio = 12.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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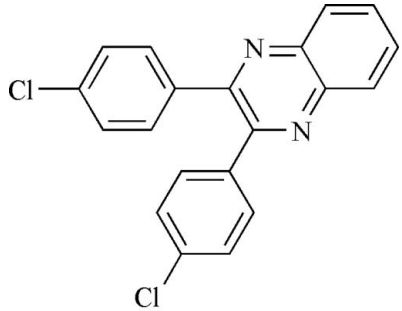
In the title compound, $C_{20}H_{12}C_{l2}N_2$, the two benzene rings make dihedral angles of 57.3 (2) and 35.0 (2)° with the quinoxaline ring system.

Comment

Quinoxaline derivatives used in organic light-emitting diodes as electron-transport materials have been explored in many studies due to their high thermal stability, outstanding mechanical properties and good film-forming ability (Kulkarni *et al.*, 2005; Fukuda *et al.*, 1996; O'Brien *et al.*, 1996). Functionalized quinoxalines also possess a wide range of biological properties, including anticancer (Lindsley *et al.*, 2005), antiviral (Loriga *et al.*, 1997) and antibacterial activities (Seitz *et al.*, 2002), and activity as kinase inhibitors (He *et al.*, 2003). Here, we report the synthesis and crystal structure of the title compound, (I).



(I)

In the molecular structure of (I), the two benzene rings attached to the quinoxaline ring system are inclined at an angle of 64.1 (2)°. The C7,C10,C14,C15,C18,C20 and C4,C5,C6,C11,C12,C16 benzene rings make dihedral angles of 57.3 (2) and 35.0 (2)°, respectively, with the planar quinoxaline ring system.

Experimental

A suspension of 1,2-bis(4-chlorophenyl)ethane-1,2-dione (0.8 mmol) and benzene-1,2-diamine (1.0 mmol) in acetic acid (3 ml) was heated to reflux for 0.5 h. The mixture was then poured into ice–water and a white precipitate was formed. The mixture was neutralized using saturated $NaHCO_3$ solution. The resulting precipitate was filtered off, washed with water, dried and purified by recrystallization using a mixture of ethyl acetate and petroleum ether (1:5), giving the target product as white needle crystals in 99.3% yield. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform–ethanol (1:1).

Crystal data

$C_{20}H_{12}Cl_2N_2$
M_r = 351.22
Triclinic, $P\overline{1}$
a = 5.9282 (6) Å
b = 11.9737 (12) Å
c = 12.0247 (13) Å
α = 104.764 (7)°
β = 92.259 (7)°
γ = 95.778 (7)°
V = 819.29 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 298 (2) K
0.30 × 0.26 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.890, T_{max} = 0.943
4712 measured reflections
2788 independent reflections
2268 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.139
S = 1.02
2788 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C20—C19	1.482 (3)	C17—C16	1.487 (3)
N2—C19—C20	115.04 (16)	N1—C17—C16	116.33 (16)
C13—N2—C19—C20	−173.40 (15)	C8—N1—C17—C16	−174.90 (15)

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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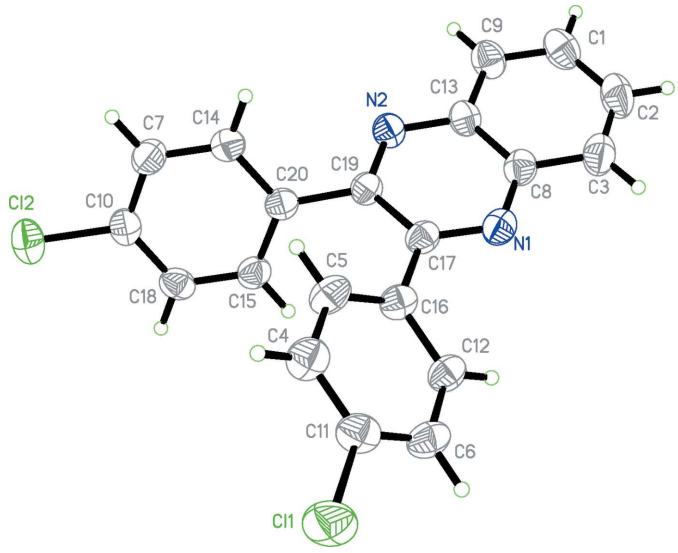

Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

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