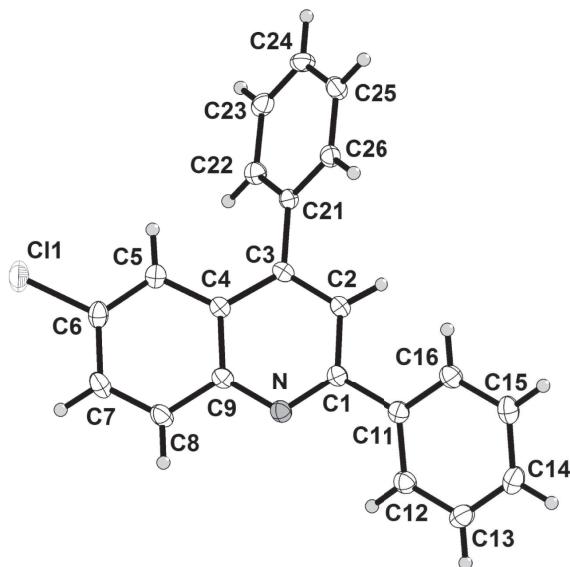


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# The crystal structure of 6-chloro-2,4-diphenylquinoline



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## Abstract

$C_{21}H_{14}ClN$ , orthorhombic,  $Pca2_1$  (No. 29),  $a = 7.6860(5)$  Å,  $b = 10.1610(5)$  Å,  $c = 19.8990(5)$  Å,  $V = 1554.1(13)$  Å<sup>3</sup>,  $Z = 4$ ,  $R_{gt}(F) = 0.0318$ ,  $wR_{ref}(F^2) = 0.0783$ ,  $T = 100(2)$  K.

CCDC no.: 1442751

The crystal structure is shown in the figure, Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

## Source of material

Synthesis protocols toward quinoline derivatives involve the use of a Brønsted acid or Lewis acid catalyst [12–20]. Preparation of these compounds under microwave conditions have also been reported [13–15]. A solution of benzaldehyde (5 mL),

**Table 1:** Data collection and handling.

Crystal:	Yellow, cuboid, size $0.389 \times 0.47 \times 0.651$ mm
Wavelength:	Mo $K\alpha$ radiation ( $0.71073$ Å)
$\mu$ :	$2.44$ cm <sup>-1</sup>
Diffractometer, scan mode:	Bruker APEX-II CCD, $\varphi$ and $\omega$ scans
$2\theta_{max}$ :	$55.99^\circ$
$N(hkl)_{measured}$ , $N(hkl)_{unique}$ :	26440, 3754
$N(param)_{refined}$ :	208
Programs:	Bruker data collection and reduction software [21], SHELX [22], Diamond [23]

**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>).

Atom	Site	x	y	z	$U_{iso}$
H(5)	4a	0.6766	-0.1534	0.6398	0.023
H(26)	4a	0.7630	0.2657	0.6155	0.022
H(2)	4a	0.5213	0.2496	0.5412	0.021
H(7)	4a	0.5322	-0.4166	0.4992	0.030
H(24)	4a	0.7423	0.2323	0.8166	0.030
H(25)	4a	0.8452	0.3381	0.7211	0.028
H(16)	4a	0.5853	0.3669	0.4501	0.025
H(15)	4a	0.5339	0.5228	0.3677	0.029
H(22)	4a	0.4723	-0.0195	0.7004	0.024
H(23)	4a	0.5519	0.0565	0.8061	0.027
H(13)	4a	0.2150	0.2696	0.2727	0.029
H(8)	4a	0.4329	-0.2502	0.4308	0.026
H(12)	4a	0.2606	0.1157	0.3568	0.025
H(14)	4a	0.3511	0.4733	0.2779	0.030

phenylacetylene (8 mL) and 4-chloroaniline (6.39 g) and  $FeCl_3 \cdot 6H_2O$  (0.68 mg) was heated (100 °C) overnight. The reaction mixture was cooled to room temperature and diluted with dichloromethane (250 mL). The organic solution was extracted with water (3 × 100 mL), dried over  $Na_2SO_4$  and evaporated *in vacuo* to yield a crude product mixture. Purification was afforded with flash chromatography on silica gel ( $R_f$  0.46; hexane:ethyl acetate = 9:1). Recrystallization from a minimum amount of dichloromethane in hexane yielded the product as faint yellow needles (2.40 g, 16%).  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta = 8.22$ –8.17 (m, 1H), 7.90 (d,  $J = 2.3$  Hz, 1H), 7.85 (s, 1H), 7.67 (dd,  $J = 9.0$ , 2.3 Hz, 1H),

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**Table 3:** Atomic displacement parameters (Å<sup>2</sup>).

Atom	Site	x	y	z	<i>U</i> <sub>11</sub>	<i>U</i> <sub>22</sub>	<i>U</i> <sub>33</sub>	<i>U</i> <sub>12</sub>	<i>U</i> <sub>13</sub>	<i>U</i> <sub>23</sub>
C(1)	4a	0.4676(2)	0.1223(2)	0.46425(9)	0.0167(8)	0.017(1)	0.0179(9)	0.0005(7)	0.0026(7)	-0.0009(7)
C(3)	4a	0.5642(2)	0.0691(2)	0.5774(1)	0.0145(8)	0.017(1)	0.0168(8)	-0.0021(7)	0.0021(7)	-0.0028(7)
C(5)	4a	0.6280(2)	-0.1710(2)	0.5980(1)	0.0192(9)	0.019(1)	0.0189(8)	0.0014(8)	0.0039(7)	0.0014(7)
N	4a	0.4495(2)	-0.0026(2)	0.44632(8)	0.0227(8)	0.0178(9)	0.0169(7)	-0.0002(7)	0.0016(6)	-0.0008(6)
C(26)	4a	0.7223(2)	0.2223(2)	0.6536(1)	0.0188(9)	0.0169(9)	0.0205(9)	0.0011(7)	0.0000(7)	-0.0004(8)
C(9)	4a	0.4961(3)	-0.0962(2)	0.4923(1)	0.0190(9)	0.018(1)	0.0170(9)	-0.0013(7)	0.0028(7)	-0.0012(8)
C(2)	4a	0.5187(2)	0.1607(2)	0.5301(1)	0.0181(8)	0.0154(9)	0.0180(8)	-0.0005(7)	0.0016(7)	-0.0019(7)
C(11)	4a	0.4301(3)	0.2240(2)	0.41211(9)	0.0197(8)	0.019(1)	0.0151(8)	0.0028(7)	0.0037(7)	-0.0012(7)
C(6)	4a	0.6191(3)	-0.2973(2)	0.5748(1)	0.025(1)	0.0174(9)	0.0220(9)	0.0029(8)	0.0063(8)	0.0039(8)
C(4)	4a	0.5627(2)	-0.0667(2)	0.55779(9)	0.0157(8)	0.0163(9)	0.0158(9)	-0.0012(7)	0.0035(7)	-0.0007(7)
C(7)	4a	0.5424(3)	-0.3293(2)	0.5126(1)	0.033(1)	0.016(1)	0.026(1)	-0.0017(9)	0.0057(8)	-0.0031(8)
C(21)	4a	0.6127(2)	0.1131(2)	0.64642(9)	0.0169(8)	0.0154(9)	0.0169(8)	0.0023(7)	-0.0003(7)	-0.0017(7)
C(24)	4a	0.7085(3)	0.2034(2)	0.7742(1)	0.029(1)	0.028(1)	0.0178(9)	0.0071(9)	-0.0066(8)	-0.0078(8)
C(25)	4a	0.7709(3)	0.2663(2)	0.7169(1)	0.023(1)	0.018(1)	0.029(1)	0.0011(8)	-0.0040(8)	-0.0049(8)
C(16)	4a	0.5106(3)	0.3473(2)	0.4147(1)	0.0226(9)	0.021(1)	0.0198(9)	0.0006(8)	0.0029(8)	-0.0029(8)
C(15)	4a	0.4806(3)	0.4408(2)	0.3652(1)	0.028(1)	0.019(1)	0.025(1)	0.0013(8)	0.0066(9)	0.0020(8)
C(22)	4a	0.5477(3)	0.0517(2)	0.7043(1)	0.0202(9)	0.020(1)	0.0197(9)	0.0006(7)	0.0014(7)	-0.0006(8)
C(23)	4a	0.5957(3)	0.0973(2)	0.7678(1)	0.027(1)	0.024(1)	0.0157(9)	0.0069(8)	0.0012(8)	0.0006(8)
C(13)	4a	0.2886(3)	0.2893(2)	0.3084(1)	0.025(1)	0.029(1)	0.0195(9)	0.0047(8)	-0.0015(8)	0.0003(8)
C(8)	4a	0.4828(3)	-0.2298(2)	0.4721(1)	0.029(1)	0.019(1)	0.0175(9)	-0.0022(8)	0.0022(8)	-0.0036(7)
C(12)	4a	0.3171(3)	0.1965(2)	0.3587(1)	0.023(1)	0.021(1)	0.0193(9)	0.0006(8)	0.0013(8)	-0.0020(8)
C(14)	4a	0.3701(3)	0.4114(2)	0.3115(1)	0.029(1)	0.024(1)	0.022(1)	0.0073(8)	0.0044(9)	0.0048(8)
Cl(1)	4a	0.70653(9)	-0.42527(5)	0.62263(3)	0.0557(4)	0.0192(2)	0.0304(3)	0.0105(2)	-0.0005(3)	0.0033(2)

7.60–7.53 (m, 2H), 7.51–7.47 (m, 1H); <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>) δ = 157.08, 148.45, 147.27, 139.22, 137.79, 132.25, 131.79, 130.49, 129.66, 129.52, 128.96, 128.88, 128.77, 127.59, 126.52, 124.53, 120.06; EIMS (70 eV) *m/z* 315 (M<sup>+</sup>, 100%).

### Experimental details

The methyl H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H = 0.95 Å and *U*<sub>iso</sub>(H) = 1.5 *U*<sub>eq</sub>(C).

### Discussion

Quinoline is an important class of alkaloid of which the basic skeleton is present in numerous natural compounds [1, 2]. A high degree of biological activity, e.g. antimalarial, antibacterial, anticancer and antioxidant, have been attributed to these structures and has found application in the pharmaceutical industry [1–6]. Their unique spectral and photochemical properties have also found application in a variety of fields such as photolytic cleavage of DNA, electrogenerated chemiluminescence and light emitting diodes [7–11].

The asymmetric unit consists of one full molecule of the title compound (see the figure). The structure is stabilized by weak π-π and CH-π interactions. The π-π interaction is observed between the phenyl ring of the quinoline and the phenyl substituent of a neighbouring molecule with the angle between the dihedral planes of 9.9° and the centroid

to centroid distance of 3.913(2) Å. The CH-π interaction is observed between the phenyl ring of the quinoline and the pyridine ring of a neighbouring molecule with a CH-centroid distance of 3.493(2) Å.

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