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2-Chloro-3-chloromethylbenzo[*h*]quinoline

Adel Beghidja,[a] Ali Benboudiaf,[a] Chahrazed Beghidja[a] and Richard Welter[b]*

[a]Laboratoire de Chimie Moléculaire, du Contrôle de l'Environnement et des Mesures Physico-chimiques, Faculté des Sciences, Département de Chimie, Université Mentouri Constantine, 25000 Algeria, and [b]Laboratoire DECMET, UMR CNRS 7513, Université Louis Pasteur, 4 rue Blaise Pascal, 67000 Strasbourg, France

Correspondence e-mail: welter@chimie.u-strasbg.fr

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.060
wR factor = 0.209
Data-to-parameter ratio = 21.4

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

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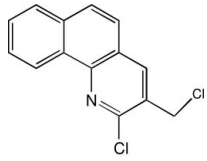
The title compound, $C_{14}H_9Cl_2N$, a derivative of benzoquinoline, is a tricyclic planar nitrogen heterocyclic system.

Comment

The molecular structure of the title compund, (I), is composed of a tricyclc planar nitrogen heterocyclic system, carrying two substituents (Cl and CH_2Cl; Fig. 1). This system displays potential biological interest (Kerry *et al.*, 1999). The crystal structure consists of planes stacked along the *b* axis. The plane-to-plane separations are 3.46 and 3.50 Å (Fig. 2).



(I)

Experimental

The title compound was prepared according to the method of Meth-Cohn *et al.* (1981). At a temperature ranging between 273 and 278 K, 0.07 mol of $POCl_3$ was added dropwise to 0.015 mol of dry *N*,*N*-dimethylformamide. Stirring was continued for 30 min, then 0.01 mol of 3-chloro-*N*-1-naphthylpropionamide, synthesized previously, was added. Stirring was continued at 353 K for 2 h and then the mixture was poured into cooled water. The brown precipitate was dried in an oven at 313 K and recrystallized from ethanol as brown needles of (I).

Crystal data

$C_{14}H_9Cl_2N$
M_r = 262.12
Triclinic, $P\overline{1}$
a = 6.9211 (10) Å
b = 8.3176 (10) Å
c = 10.6480 (10) Å
α = 79.21 (10)°
β = 76.19 (10)°
γ = 85.84 (10)°
V = 584.5 (3) Å^3
Z = 2
D_x = 1.489 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
θ = 2.5–30.0°
μ = 0.53 mm^{-1}
T = 293 (2) K
Needle, brown
0.13 × 0.05 × 0.04 mm

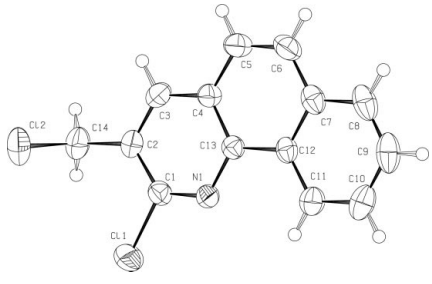


Figure 1
Molecular structure of (I). Displacement ellipsoids are shown at the 50% probability level.

Data collection

Enraf–Nonius CAD-4 diffractometer	$\theta_{max} = 30.0°$
$\theta/2\theta$ scans	$h = -9 \rightarrow 9$
Absorption correction: none	$k = 0 \rightarrow 11$
3498 measured reflections	$l = -14 \rightarrow 14$
3288 independent reflections	2 standard reflections
2022 reflections with $I > 2\sigma(I)$	frequency: 120 min
$R_{int} = 0.085$	intensity decay: 2%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0861P)^2 + 0.6126P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.060$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.210$	$\Delta\rho_{max} = 0.41$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.35$ e Å^{-3}
3288 reflections	
154 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cl1—C1	1.756 (3)	N1—C1	1.302 (4)
Cl2—C14	1.799 (4)	N1—C13	1.354 (4)
C1—N1—C13	117.1 (3)	N1—C1—C2	126.6 (3)
N1—C13—C4	122.2 (3)	N1—C1—Cl1	115.0 (2)
N1—C13—C12	118.0 (3)	C2—C1—Cl1	118.4 (2)

All H atoms in (I) were positioned geometrically and allowed to ride on their parent atoms [C—H = 0.93 and 0.97 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$].

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *XCAD*4 (Harms, 1995); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*98 (Spek, 1998); software used to prepare material for publication: *SHELXL*97.

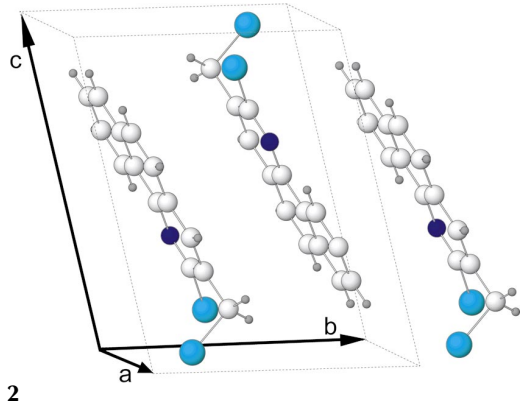


Figure 2
Packing diagram, showing the stacking of molecules of (I).

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