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Crystal Structure of *N*-8-Azanaphtylmethylene-4-chloroaniline

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Much attention has recently been concentrated on compounds obtained from heterocyclic carbaldehydes for the therapy of cancer, a major disease of our age.[1,2] Hence, in our research new Schiff bases containing different functional groups were synthesized to contribute to that class of substances, which are now being tried as anti-cancer reagents. This report describes the crystal structure of a related compound.

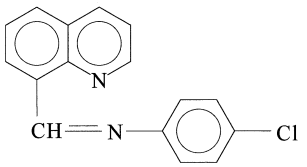


Fig. 1 Chemical diagram of *N*-8-azanaphtylmethylene-4-chloroaniline.

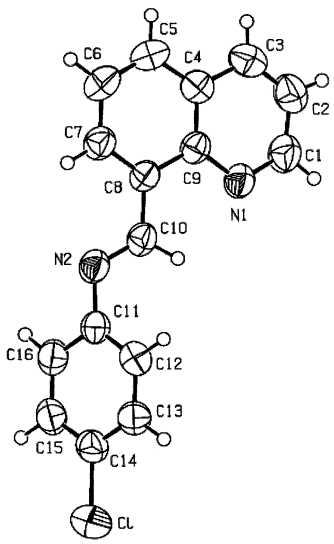


Fig. 2 Molecular geometry and the numbering scheme for the title compound. The displacement ellipsoids are plotted at the 50% probability level.

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A summary of the key crystallographic information is given in Table 1. Data collection was carried out using a Siemens SMART CCD diffractometer. The data collection was covered over a hemisphere of reciprocal space by a combination of three sets of exposures; each set had a different φ angle (0, 88 and 180˚) for the crystal and each exposure of 10 s covered 0.3˚ in ω. The crystal-to-detector distance was 4 cm and the detector swing angle was –35˚. Coverage of the unique set is over 99%

Table 1 Crystal and experimental data

Formula: $C_{16}H_{11}ClN_2$	
Formula weight = 266.72	
Crystal system: monoclinic	
Space group: $P2_1/c$ (No. 14)	$Z = 4$
a = 10.0848(6)Å	
b = 11.0341(7)Å	β = 103.497(2)˚
c = 12.1001(7)Å	
V = 1309.3(1)Å^3	
D_x = 1.353 g/cm^3	
μ (Mo K_α) = 0.3 mm^{-1}	
T = 293 K	
Color: light yellow	
F(0 0 0) = 552	
Crystal size = 0.08 × 0.38 × 0.48 mm	
Radiation: Mo K_α	
T_{max} and T_{min} = 0.9781/0.8784	
R = 0.0575	
wR = 0.1538	
No. of reflections used = 2994	($I \geq 2\sigma(I)$)
No. of parameters = 217	
Goodness-of-fit = 1.02	
$(\Delta/\sigma)_{max}$ = 0.00	
$\Delta\rho_{max}$ = 0.18 eÅ^{-3}	
$\Delta\rho_{min}$ = –0.23 eÅ^{-3}	
Measurements: SMART CCD diffractometer	
Program system: SAINT[8]	
Absorption correction: Empirical using SADABS[9]	
Structure determination: SHELXTL	
Treatment of hydrogen atoms: difference Fourier map and refined isotropically	
Refinement: full matrix least-squares	

Table 2 Atomic coodinates and equivalent isotropic displacement paremeters ($Å^2 \times 10^3$) for $C_{16}H_{11}ClN_2$

Atom	*x*	*y*	*z*	U_{eq}
Cl	0.5596(9)	0.9980(1)	0.2127(8)	0.093(1)
N1	1.1517(2)	0.8160(2)	0.8349(2)	0.063(1)
N2	0.9123(2)	0.6722(2)	0.5527(2)	0.060(1)
C1	1.2163(4)	0.8618(3)	0.9331(3)	0.074(1)
C2	1.3037(4)	0.7969(4)	1.0186(3)	0.077(1)
C3	1.3252(3)	0.6795(4)	1.0020(3)	0.072(1)
C4	1.2589(3)	0.6229(3)	0.8984(3)	0.057(1)
C5	1.2724(3)	0.4994(3)	0.8760(3)	0.066(1)
C6	1.2015(3)	0.4503(3)	0.7764(3)	0.068(1)
C7	1.1140(3)	0.5215(3)	0.6967(3)	0.061(1)
C8	1.0977(3)	0.6424(2)	0.7145(2)	0.053(1)
C9	1.1715(3)	0.6962(2)	0.8175(2)	0.051(1)
C10	1.0041(3)	0.7174(3)	0.6314(3)	0.057(1)
C11	0.8309(3)	0.7510(2)	0.4721(2)	0.054(1)
C12	0.8841(3)	0.8477(3)	0.4242(3)	0.059(1)
C13	0.8023(3)	0.9199(3)	0.3435(3)	0.062(1)
C14	0.6651(3)	0.8945(3)	0.3117(2)	0.062(1)
C15	0.6094(3)	0.7983(3)	0.3574(3)	0.066(1)
C16	0.6932(3)	0.7263(3)	0.4366(3)	0.064(1)

$U_{eq} = (1/3)\,\Sigma_i\Sigma_j U_{ij}(a_i^* a_j^*)(\boldsymbol{a}_i \cdot \boldsymbol{a}_j)$.

Table 3 Selected bond lengths (A) and bond angles (˚) for $C_{16}H_{11}ClN_2$

Cl - C14	1.743(3)	N2 - C10	1.265(4)
N1 - C1	1.315(4)	N2 - C11	1.417(3)
N1 - C9	1.361(3)	C8 - C10	1.464(4)

C1 - N1 - C9	117.0(2)	C9 - C8 - C10	119.1(2)
C10 - N2 - C11	118.7(2)	N1 - C9 - C8	118.4(2)
N1 - C1 - C2	124.6(3)	N2 - C10 - C8	122.3(3)
C3 - C4 - C5	123.4(3)	Cl - C14 - C13	119.0(2)
C7 - C8 - C10	121.7(3)	Cl - C14 - C15	119.5(2)

Table 4 Possible hydrogen bond lengths (Å) and angles (˚)

D – H (Å)		H...A (Å)		D...A (Å)		D – H...A (°)
C7 – H7	0.91(3)	H7...N2	2.57(3)	O7...N2	2.878(4)	101(2)
C10 – H10	0.96(2)	H10...N1	2.42(2)	C10...N1	2.784(4)	103(2)

complete. The crystal decay was monitored by repeating thirty initial frames at the end of the data collection, and was found to be negligible.

The structure was solved by direct methods and refined by least-squares on F^2 by using the SHELXTL software package.[3] All H-atoms were located from a difference Fourier map and refined isotropically. The final $R(F) = 0.0575$ and $wR(F^2) = 0.1538$ with the weighting scheme $w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 0.1540P]$, where $P = (F_o^2 + 2F_c^2)/3$.

The atomic coordinates and equivalent isotropic displacement parameters with the estimated standard deviations for all atoms except H are listed in Table 2; selected bond lengths and bond angles are given in Table 3.

The bond lenghts are normal;[4,5] the N1–C1 and C2–C3 bonds indicate some double-bond character.[6] The quinoline and rings are planar. The dihedral angle between the quinoline and phenyl ring is 61.8(1)˚. In the crystal lattice, presumable hydrogen bonds exist at the values given Table 4.[7]

Acknowledgements

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