Crystal structure of *N*-(4-chlorobenzylidene)-1-adamantylamine, $C_{17}H_{20}ClN$, *a Schiff base*

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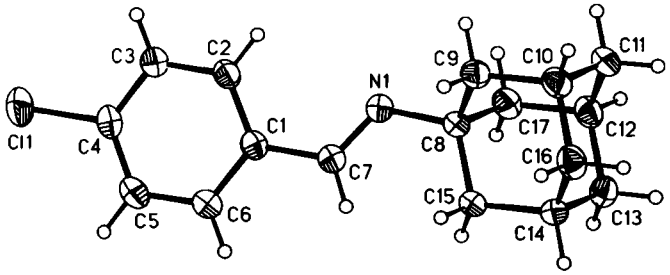

Abstract

$C_{17}H_{20}ClN$, monoclinic, *C*12/*c*1 (no. 15), $a = 27.444(6)$ Å, $b = 6.579(1)$ Å, $c = 16.574(3)$ Å, $\beta = 106.89(3)°$, $V = 2863.5$ Å^3, $Z = 8$, $R_{gt}(F) = 0.045$, $wR_{ref}(F^2) = 0.125$, $T = 293$ K.

Source of material

A mixture of adamantaneamine (0.15 g, 1 mmol) and 4-chlorobenzaldehyde (0.14 g, 1 mmol) in 30 mL ethanol (abs) was stirred and refluxed for 2 h, and then a colorless solution was formed. Single crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation of the solvent after 5 d.

Discussion

Schiff bases form an important class of compounds and find various applications. They are used as catalysts and stabilizers in polymers, pigments and dyes, photography and various biological systems. Besides, some Schiff bases have been used as analytical reagents, inhibitors against corrosion and flocculates. Otherwise, Schiff bases find application in many other fields of fundamental and applied science research. The characterization of several Schiff base ligands resulting from the condensation of salicylaldehyde, 2-hydroxy-1-naphthaldehyde and 3-hydroxy-2-naphthaldehyde with 1-adamantaneamine, i.e. *N*-(1-adamantyl)-salicylaldamine, 2-[(1-adamantyl)iminomethyl]-3-naphthol, *N*-(1-adamantanemethyl)-salicylaldamine was reported in [1]. Herein we will report the structure of a new Schiff base. The bond length for C=N [1.266(2) Å] and the bond length between the C1 atom of the aromatic ring and the N1 atom of the imine group [1.474(2) Å] correspond to a conjugated C=N group [1.270 Å – 1.296 Å] and C_{aryl}—N(=C) bond length [1.476 Å], respectively [1]. The carbon atoms of adamantine group are sp^3 hybridized with C–C–C angles ranging between 108.6(1)° and 110.4(1)°.

Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.29 × 0.40 × 0.50 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.53 cm^{-1}
Diffractometer, scan mode:	Rigaku R-AXIS RAPID IP, ω
$2\theta_{max}$:	54.96°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	13428, 3275
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2779
$N(param)_{refined}$:	172
Programs:	SHELXS-97 [2], SHELXL-97 [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2)	8*f*	0.0056	0.0354	0.0801	0.056
H(3)	8*f*	0.0774	0.1070	0.0391	0.059
H(5)	8*f*	0.0716	0.6882	0.1102	0.064
H(6)	8*f*	–0.0009	0.6158	0.1498	0.062
H(7)	8*f*	–0.0647	0.3767	0.1706	0.055
H(9A)	8*f*	–0.0888	–0.1034	0.2502	0.061
H(9B)	8*f*	–0.1069	–0.2282	0.1660	0.061
H(10)	8*f*	–0.1600	–0.3037	0.2518	0.065
H(11)	8*f*	–0.1991	–0.3150	0.1044	0.068
H(11B)	8*f*	–0.2392	–0.2451	0.1499	0.068
H(12)	8*f*	–0.2438	–0.0275	0.0343	0.064
H(13A)	8*f*	–0.2619	0.1258	0.1515	0.071
H(13B)	8*f*	–0.2363	0.2863	0.1064	0.071
H(14)	8*f*	–0.1968	0.2990	0.2532	0.065
H(15A)	8*f*	–0.1437	0.3735	0.1671	0.056
H(15B)	8*f*	–0.1113	0.2687	0.2507	0.056
H(16A)	8*f*	–0.2105	–0.0429	0.2842	0.071
H(16B)	8*f*	–0.1527	0.0112	0.3228	0.071
H(17A)	8*f*	–0.1725	0.1727	0.0330	0.062
H(17B)	8*f*	–0.1583	–0.0585	0.0324	0.062

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	8*f*	0.13603(2)	0.45740(8)	0.04388(3)	0.0582(3)	0.0799(3)	0.0890(3)	–0.0183(2)	0.0341(2)	0.0029(2)
N(1)	8*f*	–0.07661(4)	0.1117(2)	0.12377(8)	0.0435(6)	0.0471(6)	0.0559(7)	–0.0033(5)	0.0183(5)	–0.0053(5)
C(1)	8*f*	–0.00541(5)	0.3182(2)	0.11857(8)	0.0408(6)	0.0461(7)	0.0426(7)	–0.0048(5)	0.0083(5)	0.0001(5)
C(2)	8*f*	0.01868(5)	0.1667(2)	0.08584(9)	0.0420(6)	0.0443(7)	0.0514(7)	–0.0072(5)	0.0099(5)	–0.0018(6)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(3)	8*f*	0.06174(5)	0.2084(2)	0.06173(9)	0.0440(7)	0.0501(7)	0.0526(8)	–0.0029(6)	0.0129(6)	–0.0016(6)
C(4)	8*f*	0.08109(5)	0.4044(2)	0.07187(9)	0.0408(6)	0.0572(8)	0.0444(7)	–0.0084(6)	0.0085(5)	0.0053(6)
C(5)	8*f*	0.05823(6)	0.5573(2)	0.1043(1)	0.0540(8)	0.0459(7)	0.0573(8)	–0.0131(6)	0.0116(6)	0.0018(6)
C(6)	8*f*	0.01485(6)	0.5137(2)	0.1277(1)	0.0516(8)	0.0451(7)	0.0568(8)	–0.0054(6)	0.0152(6)	–0.0048(6)
C(7)	8*f*	–0.05242(5)	0.2773(2)	0.14180(9)	0.0435(7)	0.0452(7)	0.0490(7)	–0.0032(6)	0.0138(5)	–0.0030(6)
C(8)	8*f*	–0.12364(5)	0.0786(2)	0.14746(9)	0.0408(6)	0.0366(6)	0.0493(7)	–0.0029(5)	0.0147(5)	–0.0028(5)
C(9)	8*f*	–0.11622(5)	–0.1200(2)	0.1984(1)	0.0481(7)	0.0406(7)	0.0634(9)	0.0014(6)	0.0139(6)	0.0038(6)
C(10)	8*f*	–0.16527(6)	–0.1773(2)	0.2191(1)	0.0567(8)	0.0425(7)	0.0647(9)	–0.0051(6)	0.0194(7)	0.0077(6)
C(11)	8*f*	–0.20801(6)	–0.2069(2)	0.1373(1)	0.0556(8)	0.0448(7)	0.072(1)	–0.0140(6)	0.0230(7)	–0.0100(7)
C(12)	8*f*	–0.21626(6)	–0.0088(2)	0.0867(1)	0.0438(7)	0.0552(8)	0.0563(8)	–0.0096(6)	0.0056(6)	–0.0041(7)
C(13)	8*f*	–0.23063(5)	0.1609(2)	0.1386(1)	0.0414(7)	0.0525(8)	0.084(1)	0.0010(6)	0.0183(7)	0.0004(8)
C(14)	8*f*	–0.18767(5)	0.1902(2)	0.2199(1)	0.0504(8)	0.0462(7)	0.072(1)	–0.0067(6)	0.0290(7)	–0.0167(7)
C(15)	8*f*	–0.13855(5)	0.2476(2)	0.19895(9)	0.0445(7)	0.0393(6)	0.0568(8)	–0.0062(5)	0.0170(6)	–0.0088(6)
C(16)	8*f*	–0.17960(6)	–0.0070(3)	0.2705(1)	0.0598(9)	0.068(1)	0.0559(9)	–0.0162(8)	0.0243(7)	–0.0056(7)
C(17)	8*f*	–0.16721(6)	0.0484(2)	0.06583(9)	0.0520(8)	0.0527(8)	0.0481(8)	–0.0082(6)	0.0125(6)	–0.0032(6)

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