Crystal structure of *N,N'*-bis(salicylidene)-1,10-decanediamine, $C_{10}H_{20}(NCHC_6H_4OH)_2$

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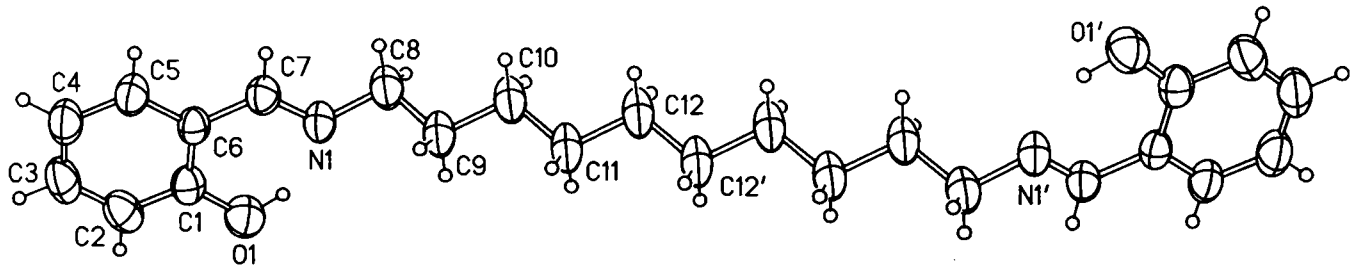

Abstract

$C_{24}H_{32}N_2O_2$, monoclinic, *C*12/*c*1 (no. 15), a = 46.409(9) Å, b = 4.800(1) Å, c = 9.987(2) Å, β = 98.10(3)°, V = 2202.4 Å^3, Z = 4, $R_{gt}(F)$ = 0.047, $wR_{ref}(F^2)$ = 0.142, T = 296 K.

Source of material

A mixture solution of 1,10-decanediamine (1.0 mmol, 0.172 g) and salicylaldehyde (2.0 mmol, 0.244g) in 30 mL methanol was stirred for 30 min at room temperature. Yellow precipitate was formed, filtered, washed with methanol and dried in air. After the product (0.095 g, 0.25 mmol) was dissolved in methanol (20 mL), yellow single crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation after 15 d.

Experimental details

The H atoms bonded to the C atoms were positioned geometrically and refined using riding models with C—H distances of 0.97 Å (aliphatic) or 0.93 Å (aromatic) and U_{iso}(H) = 1.2U_{eq}(C). The H atom bonded to the O atom was located from a Fourier difference map and refined freely.

Discussion

Schiff bases form an important class of compounds, and interest in Schiff bases and their complexes has increased greatly during recent years due to their potential and developed applications in the fields of conducting and magnetic materials, dyes, non-linear optics, catalysis, analytical chemistry, biochemical research and agriculture [1-3]. In the course of studying such compounds, we synthesized the new Schiff base, *N,N'*-bis(salicylidene)-1,10-decanediamine, and determined its crystal structure.

The ten carbon atoms of 1,10-decanediamine are approximately coplanar, with a maximum deviation of 0.049 Å for C8 from the ten-atom best plane. The twist in the molecule occurs at atom N1, with the C9–C8–N1–C7 torsion angle of 122.8(2)°. Two pyridyl rings are parallel to each other with an interplanar spacing of 5.104(1) Å. An inspection of possible hydrogen bonds indicate an intramolecular O1–H1···N1 hydrogen bonding interaction with a distance of 2.573(2) Å. Two six-membered rings defined by C1/C6/C7/N1/H1/O1 are formed because of the existence of this hydrogen bond. Additionally, there are π-π interactions between the adjacent molecules, and the shortest distance between two adjacent planes of pyridyl rings is only 3.325(3) Å.

Table 1. Data collection and handling.

Crystal:	yellow block, size 0.20 × 0.24 × 0.32 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.73 cm^{-1}
Diffractometer, scan mode:	Rigaku R-axis RAPID & Mercury CCD, ω
$2\theta_{max}$:	54.92°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9043, 2441
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1042
$N(param)_{refined}$:	132
Programs:	SHELXS-97 [4], SHELXL-97 [5], CrystalStructure [6]

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

Atom	Site	x	y	z	U_{iso}
H(2A)	8*f*	0.1829	0.6287	–0.0553	0.128
H(3A)	8*f*	0.2301	0.5128	0.0209	0.138
H(4A)	8*f*	0.2411	0.1795	0.1822	0.137
H(5A)	8*f*	0.2042	–0.0466	0.2686	0.118
H(7A)	8*f*	0.1527	–0.1389	0.2742	0.101
H(8A)	8*f*	0.1090	–0.2462	0.2926	0.122
H(8B)	8*f*	0.0882	–0.2167	0.1554	0.122
H(9A)	8*f*	0.0701	0.1999	0.2316	0.123
H(9B)	8*f*	0.0908	0.1686	0.3689	0.123
H(10A)	8*f*	0.0462	–0.2148	0.2828	0.130
H(10B)	8*f*	0.0656	–0.2202	0.4242	0.130
H(11A)	8*f*	0.0244	0.1957	0.3410	0.132
H(11B)	8*f*	0.0442	0.1955	0.4816	0.132
H(12A)	8*f*	0.0013	–0.2081	0.4022	0.134
H(12B)	8*f*	0.0208	–0.2051	0.5432	0.134
H(1)	8*f*	0.1252(4)	0.328(4)	0.059(2)	0.118(7)

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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}
C(1)	8*f*	0.16461(4)	0.3570(4)	0.0622(2)	0.081(1)	0.097(1)	0.077(1)	−0.005(1)	0.0205(9)	−0.011(1)
C(2)	8*f*	0.18706(5)	0.4916(4)	0.0104(2)	0.122(2)	0.106(1)	0.100(1)	−0.020(1)	0.042(1)	−0.004(1)
C(3)	8*f*	0.21513(5)	0.4220(5)	0.0561(3)	0.105(2)	0.118(2)	0.135(2)	−0.030(1)	0.060(2)	−0.026(1)
C(4)	8*f*	0.22178(4)	0.2240(5)	0.1516(2)	0.080(1)	0.120(2)	0.147(2)	−0.008(1)	0.037(1)	−0.019(2)
C(5)	8*f*	0.19967(4)	0.0896(4)	0.2027(2)	0.073(1)	0.109(1)	0.117(2)	0.0013(9)	0.027(1)	−0.005(1)
C(6)	8*f*	0.17090(3)	0.1513(3)	0.1591(2)	0.070(1)	0.086(1)	0.074(1)	−0.0016(8)	0.0209(8)	−0.0091(9)
C(7)	8*f*	0.14773(4)	0.0011(3)	0.2107(2)	0.076(1)	0.098(1)	0.082(1)	0.0003(9)	0.0215(9)	0.0035(9)
C(8)	8*f*	0.09945(3)	−0.1131(4)	0.2281(2)	0.075(1)	0.127(2)	0.108(1)	−0.011(1)	0.024(1)	0.014(1)
C(9)	8*f*	0.07943(3)	0.0657(4)	0.2963(2)	0.071(1)	0.136(2)	0.105(1)	−0.011(1)	0.028(1)	0.013(1)
C(10)	8*f*	0.05621(4)	−0.0981(4)	0.3538(2)	0.072(1)	0.143(2)	0.113(2)	−0.015(1)	0.026(1)	0.016(1)
C(11)	8*f*	0.03407(3)	0.0762(4)	0.4118(2)	0.068(1)	0.156(2)	0.109(1)	−0.016(1)	0.027(1)	0.015(1)
C(12)	8*f*	0.01119(3)	−0.0872(4)	0.4717(2)	0.068(1)	0.159(2)	0.112(2)	−0.016(1)	0.027(1)	0.016(1)
N(1)	8*f*	0.12127(3)	0.0519(3)	0.1735(1)	0.0678(9)	0.113(1)	0.088(1)	−0.0037(7)	0.0222(7)	0.0054(8)
O(1)	8*f*	0.13702(3)	0.4301(3)	0.0162(1)	0.104(1)	0.128(1)	0.100(1)	0.0004(8)	0.0143(8)	0.0247(8)

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