Crystal structure of (*E*)-1-(2-hydroxybenzylideneamino)imidazolidine-2,4-dione, $C_{10}H_9N_3O_3$

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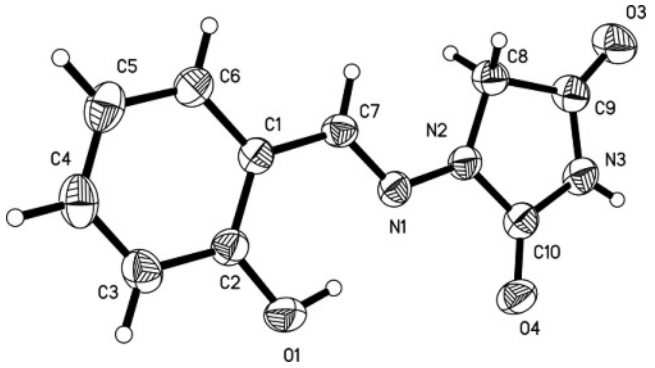

Abstract

$C_{10}H_9N_3O_3$, monoclinic, $P2_1/c$ (no. 14), a = 11.290(2) Å, b = 7.339(1) Å, c = 12.238(2) Å, β = 101.325(3)°, V = 994.3 Å^3, Z = 4, $R_{gt}(F)$ = 0.0408, $wR_{ref}(F^2)$ = 0.1209, T = 296 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.05×0.20×0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.11 cm^{-1}
Diffractometer, scan mode:	Brucker SMART CCD, φ and ω
$2\theta_{max}$:	52°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5111, 1948
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1326
$N(param)_{refined}$:	151
Programs:	SHELXS [6]

Source of material

Reagents and solvents used were of commercially available quality. The solution of 1-aminohydantoin hydrochloride (0.151 g, 1 mmol) in 1 mL of water was added to a solution containing 2-hydroxybenzaldehyde (0.122 g, 1 mmol) in 15 mL of absolute ethanol under heating and stirring. The mixture was then refluxed for 2 h. Afterwards the mixture was cooled to room temperature and the resulting solution to stand in air. On slow evaporation of the solvent, colourless block-shaped crystals were obtained after 10 days. **m.p.**: 276.9-278.3 °C. **Elemental analysis** calcd. for $C_{10}H_9N_3O_3$: C, 54.79; H, 4.14; N, 19.17; found: C, 54.73; H, 4.12; N, 19.19 %. **IR** (KBr pellet, cm^{-1}): 3213s, 3095s, 2777m, 1780s, 1728s, 1622s, 1448s, 1381s, 1277s, 1215s, 1134s, 960m, 856m, 748s, 698s, 582m.

Experimental details

The O1 and N3 H-atom were located in a difference Fourier map and refined with $U_{iso}(H) = 1.2U_{eq}$. All other H-atoms were placed in calculated positions and treated as riding: C–H = 0.93 or 0.97 Å, with $U_{iso}(H) = 1.2U_{eq}$(parent C-atom).

Discussion

The important Schiff bases have a wide range of applications in chemistry, biochemistry, medicine and technology [1, 2]. And they were still regarded as one of the most potential group of organic compounds for facile preparations of metal containing hybrid materials. The ligands containing O and N donor atoms, as analytical reagents, are increasing since they enable simple and inexpensive determinations of different metal ions [3]. As part of an ongoing study of Schiff bases containing O and N donor atoms [4], the title compound was synthesized. The X-ray diffraction analysis reveals that the compound adopts an *E* or *trans* configuration with respect to the C=N bond (N1=C7). In the molecule there is an intramolecular O–H···N hydrogen bond involving the hydroxy substituent at the 2-positon of the benzene ring and the adjacent methyleneamino N atom (figure). The molecule is almost planar, the dihedral angle between the benzene ring and imidazolidine-2,4-dione moiety 3.1(1)°, which is smaller than the dihedral angle of the similar compound (8.4(1)°, between the the naphthalene ring and imidazolidine-2,4-dione mean planes) for its little steric hindrance [5]. In the crystal, pairs of N–H···O^{i} (i = –x, –y, –z+1) hydrogen bonds link molecules into inversion dimers.

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

Atom	Site	x	y	z	U_{iso}
H(3)	4*e*	0.6804	0.4529	0.7667	0.075
H(4)	4*e*	0.8460	0.4897	0.6861	0.083
H(5)	4*e*	0.8377	0.4102	0.5030	0.084
H(6)	4*e*	0.6623	0.2917	0.3997	0.071
H(7)	4*e*	0.4537	0.1935	0.3783	0.058
H(8A)	4*e*	0.3037	–0.0164	0.2973	0.067
H(8B)	4*e*	0.2497	0.1792	0.2638	0.067
H(1)	4*e*	0.414(2)	0.278(3)	0.633(2)	0.065
H(3N)	4*e*	0.014(2)	–0.023(3)	0.395(2)	0.065

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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)	4*e*	0.5641(2)	0.2933(2)	0.5212(1)	0.0418(9)	0.050(1)	0.045(1)	0.0015(8)	0.0043(8)	0.0050(8)
C(2)	4*e*	0.5711(2)	0.3442(3)	0.6323(1)	0.050(1)	0.060(1)	0.045(1)	–0.0021(9)	0.0058(8)	0.0077(9)
C(3)	4*e*	0.6765(2)	0.4185(3)	0.6930(2)	0.065(1)	0.066(1)	0.050(1)	–0.005(1)	–0.007(1)	0.007(1)
C(4)	4*e*	0.7752(2)	0.4414(3)	0.6445(2)	0.048(1)	0.068(1)	0.081(2)	–0.003(1)	–0.010(1)	0.008(1)
C(5)	4*e*	0.7705(2)	0.3939(3)	0.5354(2)	0.043(1)	0.073(2)	0.095(2)	0.002(1)	0.015(1)	0.005(1)
C(6)	4*e*	0.6656(2)	0.3219(3)	0.4741(2)	0.048(1)	0.066(1)	0.065(1)	0.0008(9)	0.0158(9)	–0.003(1)
C(7)	4*e*	0.4555(2)	0.2187(2)	0.4530(1)	0.047(1)	0.055(1)	0.0415(9)	0.0014(8)	0.0081(8)	0.0005(8)
C(8)	4*e*	0.2445(2)	0.0730(3)	0.3098(2)	0.048(1)	0.069(1)	0.051(1)	0.0008(9)	0.0055(8)	–0.0040(9)
C(9)	4*e*	0.1185(2)	–0.0062(3)	0.2870(2)	0.047(1)	0.073(1)	0.057(1)	0.002(1)	0.0007(9)	–0.003(1)
C(10)	4*e*	0.1609(2)	0.0820(3)	0.4701(2)	0.043(1)	0.063(1)	0.053(1)	–0.0014(8)	0.0028(9)	0.0063(9)
N(1)	4*e*	0.3619(1)	0.1872(2)	0.4946(1)	0.0410(8)	0.0566(9)	0.0459(8)	–0.0046(7)	0.0029(6)	0.0029(7)
N(2)	4*e*	0.2605(1)	0.1215(2)	0.4267(1)	0.0422(8)	0.066(1)	0.0472(8)	–0.0078(7)	0.0072(7)	–0.0016(7)
N(3)	4*e*	0.0770(1)	0.0109(3)	0.3835(1)	0.0394(8)	0.080(1)	0.059(1)	–0.0083(8)	0.0038(8)	0.0027(9)
O(1)	4*e*	0.4763(1)	0.3223(2)	0.6841(1)	0.071(1)	0.109(1)	0.0432(8)	–0.0216(9)	0.0129(7)	–0.0029(8)
O(3)	4*e*	0.0656(1)	–0.0711(3)	0.2008(1)	0.0581(9)	0.122(2)	0.068(1)	–0.0080(9)	–0.0035(8)	–0.0237(9)
O(4)	4*e*	0.1493(1)	0.1049(2)	0.5656(1)	0.0535(8)	0.104(1)	0.0520(8)	–0.0150(8)	0.0122(7)	0.0028(8)

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