Yang Liguo*, Zhang Zhen, Niu Yongsheng, Wang Fang and Tian Dayong

The crystal structure of (*E*)-2-((2-hydroxy-4-ethoxybenzylidene)amino)-2-methylpropane-1,3-diol monohydrate, C₁₃H₂₁NO₅

Table 1: Data collection and handling.

Crystal:	White block
Size:	0.08 × 0.06 × 0.04 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.10 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	27.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9354, 3143, 0.036
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2409
$N(\text{param})_{\text{refined}}$:	179
Programs:	Bruker [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.32117(10)	0.4935(2)	0.0442(3)	0.0536(5)
N1	0.43692(12)	0.2560(2)	0.5309(3)	0.0460(6)
H1	0.4349	0.3422	0.4877	0.055*
C1	0.2754(2)	0.6969(4)	−0.1012(6)	0.0808(12)
H1A	0.2675	0.7433	0.0036	0.121*
H1B	0.2409	0.7266	−0.1780	0.121*
H1C	0.3191	0.7255	−0.1425	0.121*
C2	0.27328(17)	0.5343(4)	−0.0805(5)	0.0661(10)
H2A	0.2281	0.5037	−0.0481	0.079*
H2B	0.2846	0.4865	−0.1841	0.079*
O2	0.39892(9)	0.43605(19)	0.3015(3)	0.0483(5)
O3	0.47065(10)	0.5140(2)	0.6989(3)	0.0576(6)
H3	0.5095	0.5425	0.7164	0.086*
C3	0.32237(13)	0.3513(3)	0.0962(4)	0.0451(6)
C4	0.28725(16)	0.2370(4)	0.0268(5)	0.0601(9)
H4	0.2599	0.2540	−0.0648	0.072*
O4	0.59782(11)	0.2682(2)	0.7561(3)	0.0592(6)
H4A	0.6012	0.3559	0.7782	0.089*
C5	0.29200(17)	0.0944(4)	0.0922(5)	0.0660(10)
H5	0.2682	0.0180	0.0427	0.079*
O5	0.5925(3)	0.2072(4)	0.0964(5)	0.1091(12)
H5A	0.5987	0.2280	−0.0049	0.164*
H5B	0.5830	0.2890	0.1414	0.164*
C6	0.33100(15)	0.0669(3)	0.2269(5)	0.0563(8)
H6	0.3337	−0.0279	0.2693	0.068*
C8	0.36506(12)	0.3274(3)	0.2359(4)	0.0414(6)
C7	0.36767(13)	0.1829(3)	0.3032(4)	0.0442(6)
C9	0.40445(14)	0.1545(3)	0.4519(4)	0.0459(7)
H9	0.4051	0.0593	0.4935	0.055*
C10	0.47687(15)	0.2455(3)	0.6841(4)	0.0460(7)
C11	0.46158(19)	0.1078(4)	0.7820(5)	0.0683(10)

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Abstract

C₁₃H₂₁NO₅, orthorhombic, *Pca*2₁ (no. 29), *a* = 19.718(8) Å, *b* = 9.102(4) Å, *c* = 8.091(4) Å, *V* = 1452.1(11) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0452, *wR*_{ref}(*F*²) = 0.1289, *T* = 298 K [1–3].

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title molecule was synthesized from the reaction of *o*-vanillin (100 mg, 0.65 mmol) and 2-amino-2-methylpropane-1,3-diol (70 mg, 0.65 mmol) according to the procedure reported earlier [4]. Yield (0.012 g, 82%).

*Corresponding author: Yang Liguo, College of Chemistry and Environmental Engineering, Anyang Institute of Technology, Anyang 455000, Henan, P.R. China, e-mail: lgyang@ayit.edu.cn. <https://orcid.org/0000-0003-4899-8298>

Zhang Zhen, Niu Yongsheng, Wang Fang and Tian Dayong: College of Chemistry and Environmental Engineering, Anyang Institute of Technology, Anyang 455000, Henan, P.R. China

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H11A	0.4145	0.1066	0.8117	0.102*
H11B	0.4888	0.1064	0.8803	0.102*
H11C	0.4718	0.0230	0.7160	0.102*
C12	0.55189(16)	0.2497(3)	0.6248(4)	0.0512(8)
H12A	0.5623	0.1589	0.5675	0.061*
H12B	0.5575	0.3298	0.5469	0.061*
C13	0.45912(16)	0.3814(3)	0.7855(4)	0.0531(7)
H13A	0.4117	0.3765	0.8172	0.064*
H13B	0.4860	0.3816	0.8859	0.064*

Experimental details

The H atoms were geometrically placed (C–H = 0.95–0.98 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5 U_{\text{eq}}(\text{C})$. The oxygen atom of the water molecules has a larger ellipsoid due to the weak interactions with its neighborhood.

Comment

o-Hydroxy Schiff bases are a group of organic compounds, introduced into coordination chemistry as ligands. Some Schiff base compounds show photochromism and thermochromism in the solid state by proton transfer from the hydroxy O atom to the imine N atom. From the viewpoint of crystallography, *o*-hydroxy Schiff bases are of interest to the intramolecular hydrogen bond(s). *o*-Hydroxy – Schiff base compounds display two possible tautomeric forms, the phenol-imine and keto-amine form, and two types of intramolecular H-bonds are observed in Schiff bases: O–H···N in phenol-imine and N–H···O in keto-amine tautomers.

A new *o*-hydroxy schiff base was synthesized. Many similar Schiff bases were reported [4–7]. The title compound crystallizes in the orthorhombic space group *Pca*2₁ with four formula units in the unit cell. The bond lengths of N1–C10, C12–O4 and C13–O3 are 1.472, 1.406 and 1.414 Å, respectively, which are in accord with the structure reported in reference [8–20].

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