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Crystal structure of 2-((*E*)-(((*E*)-2-hydroxy-4-methylbenzylidene) hydrazineylidene)methyl)-4-methylphenol, C₁₆H₁₆N₂O₂

Table 1: Data collection and handling.

Crystal:	Brown plate
Size:	0.18 × 0.05 × 0.02 mm
Wavelength:	Cu Kα radiation (1.54184 Å)
μ :	0.71 mm ⁻¹
Diffractometer, scan mode:	XtaLAB Synergy R, ω
$\theta_{\max}$, completeness:	75.1°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	8108, 1353, 0.022
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1277
$N(\text{param})_{\text{refined}}$:	93
Programs:	CrysAlis ^{PRO} [1], SHELX [2], Olex2 [3]

$V = 680.432(17) \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.0395$, $wR_{\text{ref}}(F^2) = 0.1195$, $T = 170 \text{ K}$.

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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

2-Hydroxy-4-methylbenzaldehyde (2.72 g, 0.02 mol) was placed in 20 ml ethanol at room temperature, added into hydrazine hydrate (0.5 g, 0.01 mol) solution containing 10 ml ethanol, heated and stirred for 8 h. The mixture was cooled to room temperature, then the precipitate was removed, and the filtrate was left standing to precipitate brown crystals.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Hydrazines are organic compounds with certain biological activity [4], which are also used as dyes [5] and polymerized

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Abstract

C₁₆H₁₆N₂O₂, monoclinic, $P2_1/c$ (no. 14), $a = 8.6766(1) \text{ \AA}$, $b = 5.9039(1) \text{ \AA}$, $c = 13.3603(2) \text{ \AA}$, $\beta = 96.166(1)^\circ$,

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

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
O1	0.30212 (10)	0.90728 (14)	0.59710 (6)	0.0360 (3)
H1	0.353891	0.839600	0.558820	0.054*
N1	0.45803 (11)	0.56189 (17)	0.53242 (7)	0.0300 (3)
C1	0.27845 (13)	0.7713 (2)	0.67565 (8)	0.0279 (3)
C2	0.34302 (12)	0.55183 (19)	0.68682 (8)	0.0268 (3)
C3	0.31559 (13)	0.4268 (2)	0.77212 (9)	0.0297 (3)
H3	0.358807	0.283174	0.781215	0.036*
C4	0.15906 (13)	0.7263 (2)	0.83028 (9)	0.0316 (3)
C5	0.18639 (13)	0.8530 (2)	0.74673 (9)	0.0315 (3)
H5	0.142139	0.996017	0.737928	0.038*
C6	0.05916 (15)	0.8211 (3)	0.90552 (10)	0.0416 (4)
H6A	0.122887	0.901629	0.956921	0.062*
H6B	0.006817	0.699536	0.935541	0.062*
H6C	−0.015986	0.922749	0.872127	0.062*
C7	0.43169 (13)	0.4520 (2)	0.61207 (9)	0.0278 (3)
H7	0.470294	0.305800	0.621841	0.033*
C8	0.22629 (14)	0.5107 (2)	0.84307 (9)	0.0323 (3)
H8	0.210639	0.424396	0.899337	0.039*

monomers [6]. Especially salicylaldehyde azine, it is widely used in the study of optical properties [7, 8]. As a good ligand, Schiff base has important applications in the fields of catalysis [9] and analytical chemistry [10]. According to previous studies [11, 12], we have synthesized new ligands.

The asymmetric unit consists of one half of the title molecule, located around an inversion center of the monoclinic space group (see the Figure). The bond length of C7=N1 is 1.397 Å and N–N is 1.288 Å. The bond lengths and angles in the whole title molecule are in the expected ranges.

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