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The crystal structure of (*E*)-*N'*-((2-hydroxynaphthalen-1-yl)methylene)-2-phenylacetohydrazide, C₁₉H₁₆O₂N₂

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Abstract

C₁₉H₁₆O₂N₂, orthorhombic, *Pbca* (no. 61), $a = 12.200(2)$ Å, $b = 9.5800(19)$ Å, $c = 25.060(5)$ Å, $V = 2928.9(10)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0818$, $wR_{\text{ref}}(F^2) = 0.2438$, $T = 293(2)$ 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

The 10 mL ethanol solution containing 2-hydroxy-1-naphthaldehyde (0.1722 g, 1.0 mmol) and 2-pyrazinoic acid hydrazide (0.1381 g, 1.0 mmol) was refluxed with stirring at 70 °C for 4 h and filtered. The colourless crystals of the title compound were obtained by slow evaporation after 30 days.

Experimental details

The hydrogen atoms were positioned geometrically ($C-H = 0.93-0.97$ Å, $O-H = 0.82$ Å). Their U_{iso} values were set

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.05 × 0.04 × 0.03 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.09 mm ⁻¹
Diffractometer, scan mode:	Bruker P4, ω
θ_{max} , completeness:	27.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	23983, 3364, 0.179
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1818
$N(\text{param})_{\text{refined}}$:	197
Programs:	Bruker [1], Olex2 [2], SHELX [3], Diamond [4]

to $1.2U_{\text{eq}}$ or $1.5U_{\text{eq}}$ of the parent atoms. The non-optimal data collection gives a $R(\text{int}) > 10\%$, which systematically affects the other R factors. The atom assignment and general molecular geometry keeps unaffected.

Comment

Recently, hydrazone compounds and their metal complexes have received attention, because they have structural diversities and potential applications in antitumor activity, luminescent and antibacterial activity [5–7]. In our previous work, we have synthesized and characterized some hydrazone compounds and their metal complexes [8, 9]. In this paper, a new hydrazone compound has been synthesized and structurally characterized by single crystal X-ray diffraction.

The crystal structure of the title compound is built up by the (*E*)-*N'*-((2-hydroxynaphthalen-1-yl)methylene)-2-phenylacetohydrazide molecules. The C12–O2 and C1–O1 bond lengths are 1.198(3) Å and 1.315(3) Å, respectively, which indicates that the C12–O2 is a typical double bond. The C11–N1 and C12–N2 bond lengths are 1.247(3) Å and 1.313(3) Å, respectively, which indicates that the double bond is located at C11–N1 [10]. The angle between the plane of the phenyl ring and the best plane of the naphthyl moiety is 77.4°. In the crystal packing, the title hydrazone molecules are assembled into 3D network structure via the π - π stacking interactions not only between the phenyl groups but also between the naphthyl groups.

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C1	0.4166(2)	0.2237(3)	0.49655(10)	0.0514(7)
C2	0.4774(3)	0.1906(3)	0.45250(12)	0.0666(9)
H2A	0.506981	0.101722	0.448749	0.080*
C3	0.4938(3)	0.2864(3)	0.41522(12)	0.0657(9)
H3	0.536683	0.263587	0.385796	0.079*
C4	0.4494(2)	0.4193(3)	0.41848(11)	0.0510(7)
C5	0.4660(3)	0.5184(3)	0.37983(11)	0.0596(8)
H5	0.507412	0.495380	0.349928	0.072*
C6	0.4249(3)	0.6462(4)	0.38383(12)	0.0657(9)
H6	0.438985	0.711840	0.357370	0.079*
C7	0.3621(3)	0.6810(3)	0.42668(12)	0.0639(9)
H7	0.332185	0.770121	0.429137	0.077*
C8	0.3432(2)	0.5884(3)	0.46498(12)	0.0557(7)
H8	0.300000	0.613910	0.493949	0.067*
C9	0.3866(2)	0.4538(3)	0.46295(10)	0.0462(7)
C10	0.3715(2)	0.3534(3)	0.50285(10)	0.0449(6)
C11	0.3190(2)	0.3887(3)	0.55090(10)	0.0466(7)
H11	0.297038	0.480152	0.557239	0.056*
C12	0.2567(2)	0.2391(3)	0.66970(10)	0.0464(7)
C13	0.2378(3)	0.2949(3)	0.72337(11)	0.0622(9)
H13A	0.307655	0.317613	0.739642	0.075*
H13B	0.195427	0.380355	0.720729	0.075*
C14	0.18010(15)	0.19688(18)	0.75692(7)	0.0516(7)
C15	0.23570(14)	0.1292(2)	0.79784(8)	0.0645(9)
H15	0.309534	0.147821	0.803718	0.077*
C16	0.1810(2)	0.0336(2)	0.82996(7)	0.0776(10)
H16	0.218165	−0.011662	0.857337	0.093*
C17	0.0706(2)	0.0058(2)	0.82117(8)	0.0826(11)
H17	0.033988	−0.058156	0.842666	0.099*
C18	0.01501(15)	0.0735(2)	0.78026(9)	0.0795(11)
H18	−0.058821	0.054832	0.774377	0.095*
C19	0.06975(16)	0.1690(2)	0.74813(7)	0.0646(8)
H19	0.032546	0.214316	0.720758	0.078*
N1	0.30196(19)	0.2962(2)	0.58497(9)	0.0490(6)
N2	0.26516(19)	0.3356(2)	0.63278(9)	0.0503(6)
H2	0.247694	0.421001	0.639162	0.060*
O1	0.40632(19)	0.12283(18)	0.53182(8)	0.0629(6)
H1	0.370352	0.150874	0.557298	0.094*
O2	0.26722(19)	0.11699(18)	0.66072(8)	0.0626(6)

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