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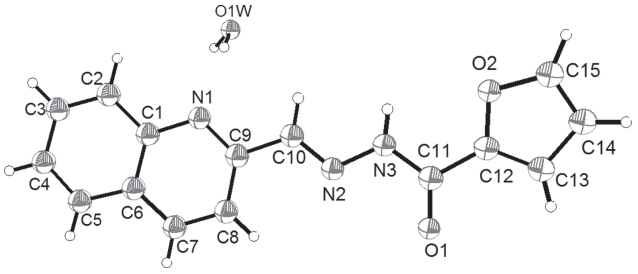
The crystal structure of (*E*)-*N'*-(quinolin-2-ylmethylene)furan-2-carbohydrazide monohydrate, $C_{15}H_{13}N_3O_3$



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Abstract

$C_{15}H_{13}N_3O_3$, triclinic, $P\bar{1}$, $a = 6.4662(13)$ Å, $b = 7.1213(14)$ Å, $c = 15.373(3)$ Å, $\alpha = 80.09(3)°$, $\beta = 88.40(3)°$, $\gamma = 74.81(3)°$, $V = 672.9(3)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0503$, $wR_{ref}(F^2) = 0.1572$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

0.156 g 2-naphthaldehyde (1.0 mmol) and 0.126 g 2-furan formylhydrazine (1.0 mmol) were dissolved in 10 mL 95% CH_3CH_2OH. The mixture was refluxed for 5 h. Then the solution was filtered. The colorless crystals of the title compound were obtained from the above filtrate by slow evaporation at room temperature for 5 days. **MS** (FAB): 282 (M + 1). **IR**: 3452 cm^{-1} (O—H and N—H), 1639 cm^{-1} (C=O), 1592 cm^{-1} (C=N). **^{1}H NMR** (ppm): 10.13 (s, 1H, N—H), 8.21 (s, 1H,—CH = N), 7.24–8.19 (s, 7H, Ar—H) 6.80–7.16 (s, 3H, furan-H). **^{13}C NMR** (ppm): 161.5 (C=O), 157.6 (C=N), 122.7, 123.5, 125.0, 125.1, 126.2, 126.6, 127.3, 127.9, 130.1, 132.9 (Ar—C).

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.18 × 0.17 × 0.16 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.10 mm^{-1}
Diffractometer, scan mode:	Bruker CCD, ω-scans
$2\theta_{max}$, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5247, 2378, 0.043
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2047
$N(param)_{refined}$:	190
Programs:	Bruker programs [1], SHELX [2], DIAMOND [3]

Experimental details

Hydrogen atoms were added using riding models. Their U_{iso} values were set to 1.2 U_{eq} of the parent atoms.

Comment

Hydrazone compounds and their complexes have been widely studied due to their facile synthesis and potential biological activities [4–8]. During recent years, many hydrazone compounds and their complexes have displayed extensive applications in luminescent probe, antibacterial, antitumor, fluorescence mark and anticonvulsant agents [9–12]. A series of hydrazone compounds and their complexes have been synthesized which show novel structure and luminescent properties [13–15].

The title compound has an almost coplanar configuration with a dihedral angle of 7.8° between the plane 1 (C1—C2—C3—C4—O1) and plane 2 (C6—C7—C8—C9—C10—C11). The crystal structure analysis shows that the title compound contains one water molecule in the structure. From the data of bond lengths, it can be seen that the C16—N1 bond length of 1.278(3) Å is shorter than that of C5—N2, indicating that the bond of C16—N1 is a double bond. And the C5—O2 bond length of 1.226(2) Å is shorter than those of C1—O1 and C4—O1, which indicates that the bond of C15—O2 is also a double bond. These findings are in excellent accordance with related compounds [16, 17].

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	0.31650(18)	0.05767(19)	0.77060(8)	0.0559(4)
O2	0.8743(2)	−0.0904(2)	0.82365(9)	0.0642(4)
N1	0.5811(2)	0.32100(18)	0.38601(8)	0.0405(4)
N2	0.4767(2)	0.16071(18)	0.60881(8)	0.0399(3)
N3	0.6043(2)	0.06659(19)	0.68175(8)	0.0409(4)
H3	0.7416	0.0353	0.6778	0.049*
C1	0.4814(2)	0.4163(2)	0.30682(10)	0.0399(4)
C2	0.6095(3)	0.4435(3)	0.23259(12)	0.0531(5)
H2	0.7578	0.3963	0.2378	0.064*
C3	0.5160(3)	0.5393(3)	0.15283(12)	0.0615(5)
H3A	0.6013	0.5548	0.1038	0.074*
C4	0.2936(3)	0.6141(3)	0.14428(13)	0.0615(5)
H4	0.2330	0.6816	0.0899	0.074*
C5	0.1653(3)	0.5894(3)	0.21419(12)	0.0542(5)
H5	0.0175	0.6391	0.2074	0.065*
C6	0.2557(3)	0.4879(2)	0.29777(11)	0.0432(4)
C7	0.1325(3)	0.4517(3)	0.37302(12)	0.0512(4)
H7	−0.0163	0.4944	0.3693	0.061*
C8	0.2319(3)	0.3542(3)	0.45109(11)	0.0482(4)
H8	0.1522	0.3278	0.5008	0.058*
C9	0.4595(2)	0.2934(2)	0.45503(10)	0.0384(4)
C10	0.5768(2)	0.1934(2)	0.53751(10)	0.0410(4)
H10	0.7258	0.1534	0.5378	0.049*
C11	0.5100(2)	0.0243(2)	0.76005(10)	0.0403(4)
C12	0.6615(3)	−0.0671(2)	0.83428(11)	0.0431(4)
C13	0.6191(3)	−0.1226(3)	0.91906(11)	0.0606(5)
H13	0.4852	−0.1185	0.9436	0.073*
C14	0.8205(4)	−0.1887(4)	0.96382(14)	0.0798(7)
H14	0.8444	−0.2396	1.0237	0.096*
C15	0.9686(3)	−0.1649(4)	0.90473(14)	0.0755(7)
H15	1.1148	−0.1945	0.9168	0.091*
O1W	0.95652(17)	−0.01165(19)	0.36709(8)	0.0558(4)
H1WA	0.8735	0.1011	0.3797	0.084*
H1WB	0.8686	−0.0437	0.3262	0.084*

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