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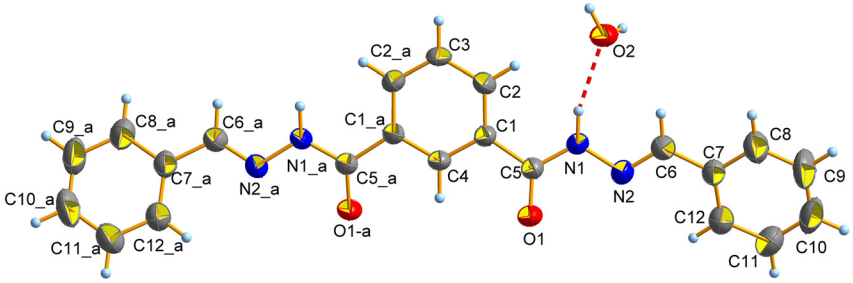
The crystal structure of N'^{1},N'^{3}-di((*E*)-benzylidene) isophthalohydrazide dihydrate, $C_{22}H_{22}N_4O_4$



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Abstract

$C_{22}H_{22}N_4O_4$, monoclinic, $C2/c$ (no. 15), a = 34.315(13) Å, b = 6.701(3) Å, c = 9.105(3) Å, β = 98.510 (4)°, V = 2070.7(13) Å^3, Z = 4, $R_{gt}(F)$ = 0.0461, $wR_{ref}(F^2)$ = 0.1413, T = 296(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.

1 Source of material

Isophthalohydrazide (10 mmol, 1.94 g) and benzaldehyde (20 mmol, 2.12 g) were dissolved in ethanol (15 mL) and the mixture was refluxed for 4 h and the resulting precipitate was collected by filtration and washed with ethanol. The product (0.5 g) was dissolved in ethanol (15 mL), and the crystals of the title compound were obtained by slow evaporation within 1 week.

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Table 1: Data collection and handling.

Crystal:	Block
Size:	0.51 × 0.45 × 0.39 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9240, 1824, 0.027
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1390
$N(param)_{refined}$:	149
Programs:	Bruker [1], SHELX [2, 3]

2 Experimental details

All hydrogen atoms were identified in difference Fourier syntheses. The U_{iso} values of all hydrogen atoms were set to 1.2 U_{eq}(C).

3 Comment

Aroylhydrazone compounds have rich biological activities, such as the treatment of tuberculosis, fungicidal activity and so on [4–7]. Meanwhile, because of their strong coordination ability, aroylhydrazone compounds are often used for metal ion detection [8–10].

Herein, a novel aroylhydrazone compound was synthesized and characterized by single-crystal X-ray diffraction [1–3]. In the crystal, the molecule exhibits crystallographic twofold axial symmetry where C(3) and C(4) are located. The title molecule is the solvtomorph of the corresponding methanol containing compound [7]. The title molecule is non-planar and the dihedral angle between rings C1–C4 and C7–C12 is 18.4 (5)°. The bond lengths of C(1)–C(5), C(5)–O(1), C(5)–N(1), N(1)–N(2), N(2)–C(6) and C(6)–C(7) are 1.4980(19), 1.2389(19), 1.3519(18), 1.3850(17), 1.278(2)

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.02778 (4)	0.0116 (2)	0.18142 (15)	0.0368 (4)
C2	0.02747 (5)	−0.1952 (2)	0.1818 (2)	0.0515 (5)
H2	0.045704	−0.265788	0.136148	0.062*
C3	0.000000	−0.2959 (3)	0.250000	0.0645 (8)
H3	0.000000	−0.436 (6)	0.250000	0.094 (10)*
C4	0.000000	0.1126 (3)	0.250000	0.0390 (5)
H4	0.000000	0.261 (4)	0.250000	0.052 (7)*
C5	0.05656 (4)	0.1350 (2)	0.11193 (16)	0.0393 (4)
C6	0.13097 (5)	0.0466 (3)	−0.10204 (18)	0.0477 (4)
H6	0.132503	−0.090757	−0.087861	0.057*
C7	0.15728 (5)	0.1438 (3)	−0.19286 (19)	0.0487 (4)
C8	0.18771 (6)	0.0347 (3)	−0.2392 (2)	0.0672 (6)
H8	0.191572	−0.097623	−0.209891	0.081*
C9	0.21231 (6)	0.1216 (4)	−0.3287 (3)	0.0809 (7)
H9	0.232901	0.048056	−0.357335	0.097*
C10	0.20652 (7)	0.3145 (4)	−0.3751 (3)	0.0801 (7)
H10	0.222996	0.371772	−0.435773	0.096*
C11	0.17610 (7)	0.4244 (3)	−0.3315 (3)	0.0795 (7)
H11	0.171917	0.555291	−0.363945	0.095*
C12	0.15199 (6)	0.3404 (3)	−0.2403 (2)	0.0643 (6)
H12	0.131903	0.416139	−0.209962	0.077*
N1	0.08100 (4)	0.03705 (19)	0.03306 (14)	0.0429 (4)
H1	0.081057	−0.091184	0.029501	0.052*
N2	0.10593 (4)	0.14748 (19)	−0.04191 (14)	0.0443 (4)
O1	0.05818 (4)	0.31847 (16)	0.12824 (14)	0.0552 (4)
O2	0.08283 (4)	−0.37552 (19)	−0.06118 (17)	0.0609 (4)
H2A	0.0743 (7)	−0.384 (4)	−0.163 (3)	0.104 (9)*
H2B	0.0790 (7)	−0.486 (5)	−0.022 (3)	0.092 (8)*

and 1.464(2) respectively. The bond angles of C(1)–C(5)–O(1), O(1)–C(5)–N(1) and C(1)–C(5)–N(1) are 121.19 (13)°, 121.67 (13)° and 117.13 (13)° [11]. In the crystal, the acyl hydrazone molecule and water molecule are connected by a hydrogen bond N(1)–H···O(2) (see the figure).

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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