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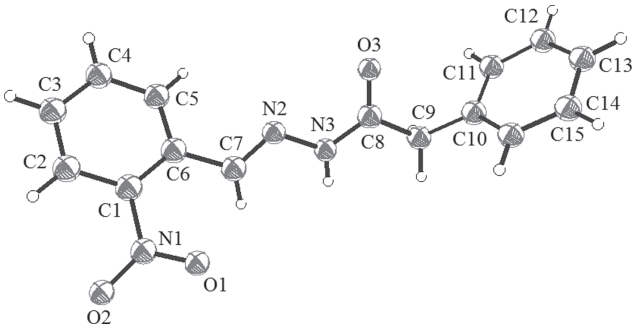
The crystal structure of *N′*-(2-nitrobenzylidene)-2-phenylacetohydrazide, $C_{15}H_{13}N_3O_3$



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Abstract

$C_{15}H_{13}N_3O_3$, orthorhombic, $P2_12_12_1$ (no. 19), $a = 8.6321(17)$ Å, $b = 12.120(2)$ Å, $c = 13.540(3)$ Å, $V = 1416.6(5)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0453$, $wR_{ref}(F^2) = 0.1141$, $T = 293(2)$ 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

0.1511 g 2-nitrobenzaldehyde (1.0 mmol) and 0.1502 g 2-phenylacetohydrazide (1.0 mmol) were dissolved in 20 mL C_2H_5OH. Then the reaction mixture was heated at 70 °C with stirring for 4 h. After cooling to room temperature, the solution was filtered and evaporated to obtain brown crystals in 13 days. Elemental analysis calc. for $C_{15}H_{13}N_3O_3$: C, 63.54, H, 4.59, N, 14.83(%); Found: C, 63.41, H, 4.78, N, 14.66(%). **EI-MS**:*m*/*z* 283.

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Table 1: Data collection and handling.

Crystal:	Block, brown
Size:	0.21 × 0.20 × 0.19 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}:	10569, 2491, 0.053
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2137
$N(param)_{refined}$:	190
Programs:	Bruker programs [1], SHELX [2], OLEX2 [3], DIAMOND [4]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	1.5219(5)	0.3756(2)	0.9957(2)	0.1168(11)
O2	1.4837(6)	0.2321(2)	1.0827(3)	0.1490(17)
O3	1.67276(18)	0.85139(14)	1.00245(14)	0.0531(5)
N1	1.5276(5)	0.3274(2)	1.0737(3)	0.0928(10)
N2	1.5573(2)	0.66140(16)	1.07404(15)	0.0449(5)
N3	1.4785(2)	0.72674(15)	1.00734(16)	0.0442(5)
H3B	1.3892	0.7069	0.9854	0.053*
C1	1.5870(4)	0.3848(2)	1.1606(2)	0.0638(8)
C2	1.6584(5)	0.3218(3)	1.2329(3)	0.0889(13)
H2A	1.6642	0.2455	1.2264	0.107*
C3	1.7202(4)	0.3731(5)	1.3137(4)	0.1012(16)
H3A	1.7679	0.3314	1.3628	0.121*
C4	1.7122(4)	0.4851(4)	1.3228(3)	0.0923(13)
H4A	1.7574	0.5197	1.3769	0.111*
C5	1.6370(3)	0.5474(3)	1.2516(2)	0.0640(8)
H5A	1.6282	0.6233	1.2603	0.077*
C6	1.5747(3)	0.4991(2)	1.1678(2)	0.0494(6)
C7	1.4966(3)	0.5689(2)	1.09399(19)	0.0469(6)
H7A	1.4060	0.5459	1.0631	0.056*
C8	1.5430(3)	0.8217(2)	0.97722(17)	0.0413(5)
C9	1.4421(3)	0.8898(2)	0.9095(2)	0.0591(8)
H9A	1.3840	0.8407	0.8667	0.071*
H9B	1.3683	0.9310	0.9490	0.071*
C10	1.5333(3)	0.9687(2)	0.84706(19)	0.0456(6)
C11	1.5631(4)	1.0745(3)	0.8793(2)	0.0619(7)
H11A	1.5242	1.0973	0.9401	0.074*
C12	1.6492(4)	1.1470(3)	0.8235(3)	0.0758(9)
H12A	1.6670	1.2182	0.8464	0.091*
C13	1.7083(4)	1.1147(3)	0.7348(3)	0.0723(10)
H13A	1.7684	1.1635	0.6981	0.087*
C14	1.6799(4)	1.0116(3)	0.6997(2)	0.0684(8)
H14A	1.7187	0.9902	0.6386	0.082*
C15	1.5918(3)	0.9376(2)	0.7562(2)	0.0595(7)
H15A	1.5727	0.8670	0.7324	0.071*

Experimental details

All hydrogen atoms were placed geometrically and refined using a riding model with U_{iso} set to 1.2 U_{eq} of the parent atom.

Comment

The title compound was characterised by elemental analysis, EI-MS and single-crystal X-ray diffraction. The two aromatic rings are not coplanar with a dihedral angle of 61.5° between ring 1 (C1—C2—C3—C4—C5—C6) and ring 2 (C10—C11—C12—C13—C14—C15). The double bond distances of C8—O3 and C7—N2 are 1.225(3) Å and 1.266(3) Å, respectively. These values are normal and are similar to those reported for related compounds [5–10]. In the crystal packing, the hydrazone molecules form infinite 1D chains along [100] linked by intermolecular N—H···O(carbonyl) hydrogen bonds.

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