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The crystal structure of 2-carboxybenzaldehyde-2-phenylacetohydrazone, $C_{16}H_{14}N_2O_3$

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.18 × 0.17 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.10 mm ⁻¹
Diffractometer, scan mode:	Bruker-CCD, ω -scans
$\theta_{\max}$, completeness:	25°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	5320, 2434, 0.043
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1848
$N(\text{param})_{\text{refined}}$:	190
Programs:	Bruker programs [1], SHELX [2, 3], DIAMOND [4]

The asymmetric unit of the title 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

An amount of 0.751 g 2-carboxybenzaldehyde (0.05 mmol) solid was added to the solution of 2-phenylacetohydrazide (0.751 g, 0.5 mmol) in 15 mL C_2H_5OH/H_2O (v:v = 2:1). The reaction mixture was stirred for 5 h at 70 °C and cooled to room temperature. The block crystals were obtained by slowly evaporating the solution at room temperature. Elemental analysis calc. for $C_{16}H_{14}N_2O_3$: C, 68.02, H, 4.96, N, 9.92(%); Found: C, 68.21, H, 4.69, N, 9.78(%). EI-MS: m/z 282.

Experimental details

Coordinates of hydrogen atoms were derived from their parent atoms. Their U_{iso} values were set to 1.2 U_{eq} of the parent atoms.

Comment

Design and synthesis of multifunctional ligands have always been our goal [5, 6]. In this paper, a new multifunctional ligand, 2-carboxybenzaldehyde-2-phenylacetohydrazone with both carboxylate group and $-C=N$ group is reported.

In the molecule of the title compound, aryl ring 1 (C1–C2–C3–C4–C5–C6) forms a dihedral angle of 113.9° with aryl ring 2 (C10–C11–C12–C13–C14–C15). The bond distances of C9–O3 and C8–N1 are 1.239(2) Å and 1.280(2) Å, respectively, which indicates that there are double bonds and their lengths are consistent with those reported in Ref. [7–11]. In the crystal

<https://doi.org/10.1515/ncrs-2017-0361>

Received January 4, 2018; accepted March 27, 2018; available online April 13, 2018

Abstract

$C_{16}H_{14}N_2O_3$, triclinic, $P\bar{1}$ (no. 2), $a = 7.7698(16)$ Å, $b = 8.3020(17)$ Å, $c = 12.197(2)$ Å, $\alpha = 92.94(3)^\circ$, $\beta = 107.03(3)^\circ$, $\gamma = 110.41(3)^\circ$, $V = 694.6(3)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0582$, $wR_{\text{ref}}(F^2) = 0.1683$, $T = 293(2)$ K.

CCDC no.: 1832886

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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}
N1	0.0770(2)	−0.1613(2)	−0.22481(13)	0.0418(4)
N2	−0.1027(2)	−0.2628(2)	−0.22069(14)	0.0452(4)
H2A	−0.1268	−0.2502	−0.1570	0.054*
C1	0.4035(3)	0.2771(2)	0.04399(16)	0.0420(5)
C2	0.4892(2)	0.2221(2)	−0.03860(15)	0.0387(5)
C3	0.6775(3)	0.3255(3)	−0.03187(18)	0.0491(5)
H3A	0.7480	0.4250	0.0249	0.059*
C4	0.7614(3)	0.2827(3)	−0.1083(2)	0.0599(6)
H4A	0.8874	0.3529	−0.1032	0.072*
C5	0.6571(3)	0.1351(3)	−0.1922(2)	0.0625(7)
H5A	0.7124	0.1067	−0.2446	0.075*
C6	0.4716(3)	0.0295(3)	−0.19910(17)	0.0512(5)
H6A	0.4048	−0.0713	−0.2549	0.061*
C7	0.3818(3)	0.0703(2)	−0.12436(15)	0.0394(5)
C8	0.1859(3)	−0.0482(2)	−0.13280(15)	0.0410(5)
H8A	0.1404	−0.0413	−0.0709	0.049*
C9	−0.2434(3)	−0.3814(3)	−0.31167(16)	0.0413(5)
C10	−0.1956(3)	−0.4234(3)	−0.41802(16)	0.0429(5)
H10A	−0.0847	−0.3263	−0.4223	0.051*
H10B	−0.3054	−0.4418	−0.4874	0.051*
C11	−0.1491(2)	−0.5858(2)	−0.41227(15)	0.0378(5)
C12	0.0233(3)	−0.5814(3)	−0.33352(17)	0.0476(5)
H12A	0.1109	−0.4774	−0.2846	0.057*
C13	0.0663(3)	−0.7282(3)	−0.32671(19)	0.0565(6)
H13A	0.1820	−0.7231	−0.2729	0.068*
C14	−0.0608(3)	−0.8830(3)	−0.39907(19)	0.0578(6)
H14A	−0.0314	−0.9824	−0.3945	0.069*
C15	−0.2321(3)	−0.8896(3)	−0.47846(19)	0.0570(6)
H15A	−0.3183	−0.9936	−0.5279	0.068*
C16	−0.2760(3)	−0.7420(3)	−0.48466(16)	0.0468(5)
H16A	−0.3922	−0.7477	−0.5381	0.056*
O1	0.53628(18)	0.38260(19)	0.13923(12)	0.0572(5)
H1	0.4824	0.4090	0.1818	0.086*
O2	0.22998(18)	0.23251(19)	0.02573(12)	0.0548(4)
O3	−0.40693(19)	−0.45740(19)	−0.30428(12)	0.0533(4)

adjacent molecules form dimers by intermolecular N—H⋯O and O—H⋯O hydrogen bonds.

Acknowledgements: This project was supported by the National Natural Science Foundation of China (No. 21171132), the Natural Science Foundation of Shandong (ZR2014BL003), the project of Shandong Province Higher Educational Science and Technology Program (J14LC01) and Science Foundation of Weifang.

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