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The crystal structure of ethyl 5,6-dihydroxybenzofuran-3-carboxylate, $C_{11}H_{10}O_5$

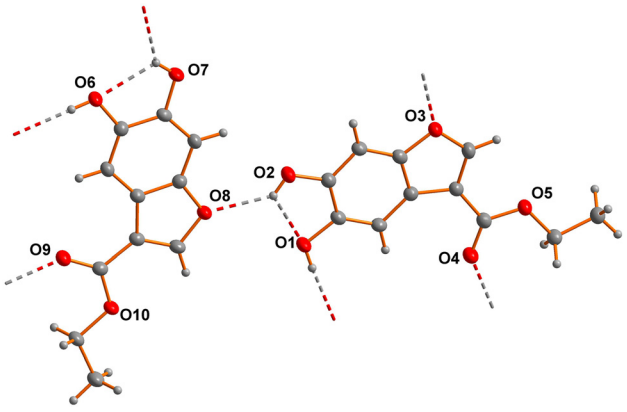

Table 1: Data collection and handling.

Crystal:	Colourless needle
Size:	0.45 × 0.05 × 0.03 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	1.03 mm^{-1}
Diffractometer, scan mode:	ROD, Synergy Custom DW system, HyPix, ω
θ_{max}, completeness:	77.1°, >99 %
N $(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	27,095, 3,873, 0.064
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3,463
$N(param)_{refined}$:	295
Programs:	Olex2,[1] SHELX[2,3]

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Abstract

$C_{11}H_{10}O_5$, triclinic, $P\bar{1}$ (no. 2), a = 8.9847(3) Å, b = 10.5228(3) Å, c = 11.2032(4) Å, α = 106.484(3)°, β = 93.420(3)°, γ = 103.646(3)°, V = 977.84(6) $Å^3$, Z = 4, $R_{gt}(F)$ = 0.0441, $wR_{ref}(F^2)$ = 0.1298, T = 293 K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of materials

In a representative experiment, 0.20 g (1 mmol) of ethyl 5,6-dihydroxybenzofuran-3-carboxylate was dissolved in 10 mL of ethyl acetate. The solution was stirred and gently heated to 50 °C to ensure complete dissolution. The clear solution was then allowed to cool to room temperature and subsequently left to slowly evaporate at ambient conditions. Crystals of the title compound were obtained within 3 days by slow evaporation of the solvent.

2 Experimental details

Reflections were measured on a four-circle diffractometer (ROD, Synergy Custom DW system, HyPix) using Cu Kα radiation (λ = 1.54184 Å). The data collection was performed using ω scans, and the data reduction was carried out using CrysAlis^{Pro} 1.171.43.98a (Rigaku OD, 2023).

The structure was solved by Direct Methods using SHELXS[2] and refined by full-matrix least-squares on F^2 using SHELXL 2018/3.[3] Non-hydrogen atoms were refined anisotropically. The hydrogen atoms were treated using a riding model with U_{iso} values set at 1.2 or 1.5 times the U_{eq} of the parent atoms.

3 Comment

Ethyl 5,6-dihydroxybenzofuran-3-carboxylate is a compound of significant interest due to its potential applications in various fields such as medicinal chemistry and organic synthesis. The presence of hydroxy groups on the benzofuran ring can further enhance these activities by providing additional sites for hydrogen bonding and other interactions.

In this study, the crystal structure of ethyl 5,6-dihydroxybenzofuran-3-carboxylate was determined to

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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}
C1	0.82920 (17)	0.23276 (16)	0.64227 (14)	0.0255 (3)
C2	0.74164 (17)	0.29189 (15)	0.73317 (14)	0.0246 (3)
C3	0.71513 (17)	0.24666 (15)	0.83643 (14)	0.0246 (3)
H3	0.659859	0.285929	0.897689	0.029*
C4	0.77601 (17)	0.13940 (15)	0.84278 (14)	0.0241 (3)
C5	0.85864 (17)	0.07629 (15)	0.75369 (14)	0.0233 (3)
C6	0.88707 (17)	0.12485 (15)	0.65060 (14)	0.0246 (3)
H6A	0.943049	0.085583	0.589944	0.030*
C7	0.89369 (17)	−0.03212 (15)	0.79640 (14)	0.0241 (3)
C8	0.83094 (18)	−0.02605 (16)	0.90450 (15)	0.0265 (3)
H8	0.836137	−0.085657	0.951097	0.032*
C9	0.97135 (17)	−0.13437 (16)	0.73090 (14)	0.0256 (3)
C10	1.05862 (18)	−0.32943 (16)	0.73220 (15)	0.0272 (3)
H10A	1.161217	−0.287341	0.717365	0.033*
H10B	0.998998	−0.387320	0.652153	0.033*
C11	1.06886 (19)	−0.41340 (16)	0.81892 (15)	0.0300 (3)
H11A	1.119865	−0.482886	0.782610	0.045*
H11B	0.966673	−0.456195	0.831437	0.045*
H11C	1.126616	−0.354886	0.898225	0.045*
C12	0.46757 (17)	0.86445 (15)	0.73289 (14)	0.0238 (3)
C13	0.49102 (17)	0.77263 (15)	0.79855 (13)	0.0235 (3)
C14	0.56077 (17)	0.66887 (15)	0.74831 (14)	0.0244 (3)
H14	0.574258	0.606395	0.789638	0.029*
C15	0.60908 (17)	0.66435 (15)	0.63246 (14)	0.0241 (3)
C16	0.58982 (16)	0.75362 (15)	0.56622 (14)	0.0235 (3)
C17	0.51608 (17)	0.85622 (15)	0.61677 (14)	0.0238 (3)
H17	0.500296	0.916654	0.573769	0.029*
C18	0.65597 (16)	0.70931 (15)	0.45089 (13)	0.0237 (3)
C19	0.70868 (18)	0.60082 (16)	0.45739 (14)	0.0268 (3)
H19	0.756807	0.553097	0.395164	0.032*
C20	0.66484 (17)	0.76987 (15)	0.34828 (14)	0.0239 (3)
C21	0.73335 (19)	0.75014 (17)	0.14374 (14)	0.0276 (3)
H21A	0.800723	0.842807	0.171291	0.033*
H21B	0.633675	0.752553	0.107466	0.033*
C22	0.8024 (2)	0.65689 (18)	0.04846 (16)	0.0353 (4)
H22A	0.815785	0.690070	−0.022705	0.053*
H22B	0.734567	0.565661	0.021781	0.053*
H22C	0.900865	0.655382	0.085440	0.053*
O1	0.84964 (14)	0.29270 (12)	0.54842 (10)	0.0308 (3)
H1	0.887304	0.246306	0.492731	0.046*
O2	0.68228 (13)	0.39553 (11)	0.72010 (10)	0.0292 (3)
H2	0.703250	0.411234	0.654572	0.044*
O3	0.75941 (12)	0.07729 (11)	0.93711 (10)	0.0265 (3)
O4	1.01935 (13)	−0.13612 (12)	0.63022 (11)	0.0308 (3)
O5	0.98364 (13)	−0.22408 (11)	0.79169 (10)	0.0275 (3)
O6	0.39448 (13)	0.95966 (11)	0.79458 (10)	0.0282 (3)
H6	0.380333	1.006932	0.750269	0.042*
O7	0.44462 (13)	0.78639 (11)	0.91463 (10)	0.0286 (3)
H7	0.401268	0.848413	0.932024	0.043*
O8	0.68306 (12)	0.56956 (11)	0.56582 (10)	0.0267 (3)
O9	0.63006 (13)	0.87628 (11)	0.35308 (10)	0.0293 (3)
O10	0.71575 (13)	0.69566 (11)	0.24911 (10)	0.0274 (3)

gain a better understanding of its molecular conformation and intermolecular interactions. The asymmetric unit of the title compound contains two molecules. The bond lengths and angles within the molecule are within the expected ranges, indicating a well-ordered structure.[4–6] There are several O-H···O hydrogen bonds (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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