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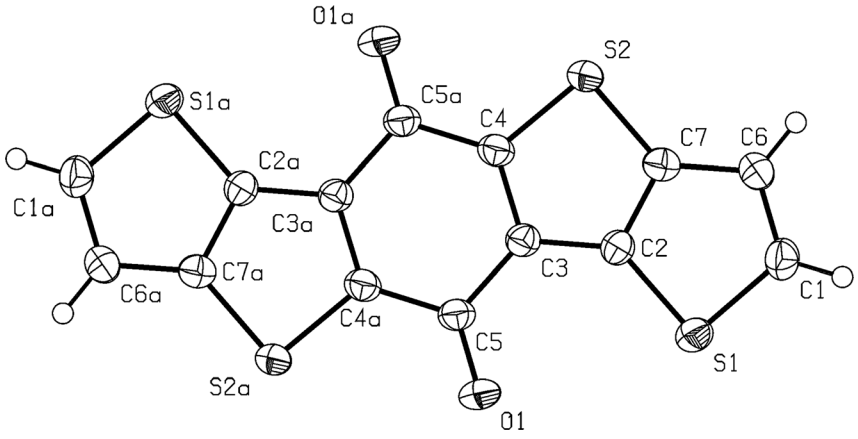
Crystal structure of dithieno[2,3-*d*:2′,3′-*d*′]benzo [1,2-*b*:4,5-*b*′]dithiophene-5,10-dione, $C_{14}H_4O_2S_4$



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Abstract

$C_{14}H_4O_2S_4$, monoclinic, $P2_1/n$ (no. 14), a = 3.85180(10) Å, b = 8.9728(2) Å, c = 18.0073(4) Å, β = 93.554(1)°, V = 621.16(3) Å^3, Z = 2, $R_{gt}(F)$ = 0.0411, $wR_{ref}(F^2)$ = 0.1091, T = 301(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.

Table 1: Data collection and handling.

Crystal:	Brown plate
Size:	0.11 × 0.10 × 0.03 mm
Wavelength:	CuKα radiation (1.54178 Å)
μ:	7.00 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	68.2°, 97 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7812, 1113, 0.060
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 989
$N(param)_{refined}$:	91
Programs:	Bruker [1], SHELX [2, 3]

1 Source of materials

1.12 g (5.3 mmol) of *N,N*-dimethylthieno[3,2-*b*]thiophene-3-carboxamide was added to 30 mL of dried THF in a flask under N_2 atmosphere. After the solution was cooled to 273 K, *n*–BuLi (1.6 M in n-hexane, 3.6 ml, 1.1 eq.) was added dropwise during 30 min. The mixture was then stirred at room temperature for 30 min. Next, it was poured into the ice/water mixture (5 g) and stirred for 3 h. Finally, the mixture was filtered and the brown precipitate washed with water (100 mL), methanol (30 mL), and THF (30 mL). The dithieno[2,3-*d*:2′,3′-*d*′]benzo[1,2-*b*:4,5-*b*′]dithiophene-5,10-dione was obtained as a brown powder (0.71 g, 81 %) after drying in a vacuum desiccator.

2 Experimental details

All hydrogen atoms were placed in idealized positions. Their U_{iso} values were set to 1.2U_{eq} of the parent atoms.

3 Comment

The dithieno[2,3-*d*:2′,3′-*d*′]benzo[1,2-*b*:4,5-*b*′]dithiophene-5,10-dione has been established to be a widely used intermediate for highly efficient solar cell materials

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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}
S1	0.5683 (2)	0.22415 (9)	0.29064 (4)	0.0325 (3)
S2	0.2353 (2)	0.32906 (9)	0.49968 (4)	0.0311 (3)
O1	0.7439 (7)	−0.1004 (3)	0.37078 (13)	0.0454 (6)
C1	0.4279 (8)	0.4063 (4)	0.28831 (18)	0.0352 (7)
H1	0.433315	0.465748	0.246101	0.042*
C2	0.4675 (7)	0.2088 (3)	0.38217 (17)	0.0272 (6)
C3	0.4935 (7)	0.0967 (3)	0.43687 (16)	0.0266 (6)
C4	0.3738 (8)	0.1465 (4)	0.50361 (17)	0.0294 (7)
C5	0.6317 (8)	−0.0560 (4)	0.42909 (17)	0.0288 (7)
C6	0.3088 (8)	0.4557 (4)	0.35309 (18)	0.0335 (7)
H2	0.223467	0.551062	0.360701	0.040*
C7	0.3324 (7)	0.3421 (4)	0.40749 (17)	0.0282 (7)

[4, 5]. Therefore, the analyzation and development of its analogs and derivatives are of increasing interest to academics.

The crystal structure of dithieno[2,3-*d*:2′,3′-*d*′]benzo[1,2-*b*:4,5-*b*′]dithiophene-5,10-dione is shown in the figure. The title molecule is located around an inversion centre. The bond lengths of C5=O1 in the title molecule is 1.226 Å, which is similar to those reported in the literature [6, 7]. Besides, all the atoms are in the same plane, and the distance between two adjacent molecules in parallel arrangement is 3.478 Å, shorter than 3.800 Å, indicating possible π–π stacking interaction between planar unsaturated cycles. The bond lengths and angles are all in the expected ranges.

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

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