2,5-di-2-thienylthiazolo[4,5-d]thiazole

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Abstract
The molecules of the title compound, C$_{12}$H$_6$N$_2$S$_4$, lie on centres of symmetry. The thiophene and thiazole rings are almost planar and their planes make a dihedral angle of 1.68 (8)$^\circ$. In the crystal structure, there is a relatively short intermolecular S···S contact distance of 3.5786 (9) Å.

Keywords
di, 2, 5, 4, thiazole, thienylthiazolo

Disciplines
Engineering | Physical Sciences and Mathematics

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2,5-Di-2-thienylthiazolo[4,5-d]-thiazole

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The molecules of the title compound, C_{12}H_{6}N_{2}S_{4}, lie on centres of symmetry. The thiophene and thiazole rings are almost planar and their planes make a dihedral angle of 1.68 (8)°. In the crystal structure, there is a relatively short intermolecular S···S contact distance of 3.5786 (9) Å.

Comment

The strong need for new ecological energy sources has resulted in a growing interest in new organic semiconducting materials, for example, those based on thiophene derivatives (for a review, see Nalva, 1997). Electrical conductivity and the band-gap (E_g) are strongly dependent on some structural parameters, including the geometry of a monomer molecule. Therefore, a detailed knowledge of the geometrical parameters (such as the planarity of the molecules, their mutual arrangement, and any intra- and intermolecular interactions) and electronic properties (e.g. the charge–density distribution) is crucial for the rational design of new materials. We performed an X-ray structural analysis of 2,5-di-2-thienylthiazolo[4,5-d]thiazole, (I) (Fig. 1), a simple model compound that could be used in electro-optically active materials. The X-ray data could then be used as the starting model for semi-empirical or ab initio calculations in molecular engineering.

![Figure 1](image)

There is a surprisingly small number of similar compounds in the Cambridge Structural Database (CSD; Allen, 2002); in the May 2002 release, we found only three thiazolo[4,5-d]thiazoles and just one compound containing the thieno–thiazole moiety. These findings further emphasize the need for more detailed structural data.

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in 11.4% of cases, contacts shorter than 3.65 Å are observed in 13.4% of cases and contacts shorter than 3.7 Å are observed in 16.4% of cases. For compounds with sulfur in a cyclic environment, these values are even higher, the respective values being 12.2, 15.3 and 18.3%. For thiazole derivatives, the fraction of compounds possessing short S· · ·S contacts is much smaller, viz. 4.2% for a 3.6 Å separation, 5.9% for a 3.65 Å separation and 8.2% for a 3.7 Å separation. Such short contacts are not found in any of the three thiazolo[4,5-c]thiazole derivatives for which the crystal structures have been reported.

The crystal packing is determined by the partial overlap of planar molecules (the distance between the mean planes of two molecules related by the center of symmetry is ca 3.6 Å) and, to some extent, by S· · ·S contacts and weak C–H· · ·S interactions (cf. Table 2).

**Experimental**

The title compound was synthesized according to the procedure of Thomas (1970) by condensation of dithiooxodiamide with 2-formyl-thiophene. Colourless prismatic crystals were grown from a methanol solution by slow evaporation.

**Crystal data**

\[
\begin{align*}
C_{13}H_6N_2S_4 & \quad D_r = 1.655 \text{ Mg m}^{-3} \\
M_r = 306.47 & \quad \text{Mo Kα radiation} \\
\text{Monoclinic, } P2_1/n & \quad \text{Cell parameters from 4325 reflections} \\
a = 6.0040 (12) \text{ Å} & \quad \theta = 4–22^\circ \\
b = 8.3580 (17) \text{ Å} & \quad \mu = 0.75 \text{ mm}^{-1} \\
c = 12.270 (3) \text{ Å} & \quad T = 100 (1) \text{ K} \\
\beta = 92.72 (3) & \quad \text{Prism, yellow} \\
V = 615.0 (2) \text{ Å}^3 & \quad Z = 2 \\
\end{align*}
\]

**Data collection**

| Kuma KM-4 CCD four-circle diffractometer | \( R_{	ext{int}} = 0.024 \) |
| 5376 measured reflections | \( \theta_{\text{max}} = 29.0^\circ \) |
| 1574 independent reflections | \( h = -8 \rightarrow 6 \) |
| 1475 reflections with \( I > 2\sigma(I) \) | \( k = -11 \rightarrow 11 \) |
| 1 | \( l = -16 \rightarrow 13 \) |

**Refinement**

**Refinement on \( F^2 \)**

\[
R(F^2 > 2\sigma(F^2)) = 0.028 \\
wR(F^2) = 0.068 \\
S = 1.10 \\
1574 reflections \\
94 parameters \\
All H-atom parameters refined
\]

**Selected geometric parameters (Å, °).**

| S1–C5 | 1.7187 (15) | S1–C4\(^iv\) | 1.7324 (14) |
| S1–C2 | 1.7287 (14) | S1–C2\(^i\) | 1.7605 (14) |
| C5–S1–C2 | 91.70 (7) | C2\(^i\)–N3–C4\(^i\) | 108.40 (12) |

C4\(^i\)–S1–C2\(^i\) | 88.38 (7) |

**Symmetry code:** (i) 1 – x, 1 – y, –z.

**Hydrogen-bonding geometry (Å, °).**

<table>
<thead>
<tr>
<th>( D - H - A )</th>
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<th>( D - H - A )</th>
</tr>
</thead>
<tbody>
<tr>
<td>C3–H3· · · S1(^i)</td>
<td>0.94 (2)</td>
<td>3.14 (2)</td>
<td>3.7296 (17)</td>
<td>122.9 (15)</td>
</tr>
<tr>
<td>C4–H4· · · S1(^ii)</td>
<td>0.97 (2)</td>
<td>3.15 (2)</td>
<td>3.8523 (17)</td>
<td>130.7 (15)</td>
</tr>
<tr>
<td>C4–H4· · · S1(^iii)</td>
<td>0.97 (2)</td>
<td>3.18 (2)</td>
<td>4.0704 (17)</td>
<td>153.4 (16)</td>
</tr>
<tr>
<td>C5–H5· · · S1(^iv)</td>
<td>0.94 (2)</td>
<td>3.10 (2)</td>
<td>3.9434 (17)</td>
<td>148.9 (16)</td>
</tr>
</tbody>
</table>

**Symmetry codes:** (ii) \( x - 1, y, z \); (iii) \( -x, -y, z \); (iv) \( \frac{1}{2} + x, y - \frac{1}{2}, -z \); (v) \( \frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z \).

Data collection: CrysAlisCCD (Kuma, 1999); cell refinement: CrysAlisCCD; data reduction: CrysAlisRed (Kuma, 1999); program(s) used to solve structure: SHELX97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: Stereochemical Workstation Operation Manual (Siemens, 1989).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV1128). Services for accessing these data are described at the back of the journal.

**References**


