Conjugated Fluorene-Thiophenes Prepared From Azomethines

Connections-I: The Effect of Electronic and Aryl Groups on the
Spectroscopic and Electrochemical Properties

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Table 1. Details of Crystal Structure Determination for 6.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>C_{23}H_{16}N_{2}S_{2}</td>
</tr>
<tr>
<td>CCSD no.</td>
<td>see remark 1</td>
</tr>
<tr>
<td>Mw (g/mol); F(000)</td>
<td>384.50 g/mol ; 800</td>
</tr>
<tr>
<td>Crystal color and form</td>
<td>Yellow plate</td>
</tr>
<tr>
<td>Crystal size (mm)</td>
<td>0.48 x 0.46 x 0.08</td>
</tr>
<tr>
<td>T (K); d\text{calcd.} (g/cm}^3</td>
<td>293 (2) ; 1.363</td>
</tr>
<tr>
<td>Crystal System</td>
<td>Orthorhombic</td>
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<tr>
<td>Space Group</td>
<td>P2_{1}2_{1}2_{1}</td>
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<tr>
<td>Unit Cell: a (Å)</td>
<td>6.0019 (16)</td>
</tr>
<tr>
<td>b (Å)</td>
<td>9.123 (3)</td>
</tr>
<tr>
<td>c (Å)</td>
<td>34.230 (9)</td>
</tr>
<tr>
<td>α (°)</td>
<td>90.000</td>
</tr>
<tr>
<td>β (°)</td>
<td>90.000</td>
</tr>
<tr>
<td>γ (°)</td>
<td>90.000</td>
</tr>
<tr>
<td>V (Å\textsuperscript{3}); Z</td>
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</tr>
<tr>
<td>θ range (°); completeness</td>
<td>2.58 – 70.03 ; 1.000</td>
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<tr>
<td>Reflections: collected / independent; R\text{int}</td>
<td>20210 / 3569 ; 0.034</td>
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<tr>
<td>μ (mm\textsuperscript{-1})</td>
<td>2.639</td>
</tr>
<tr>
<td>R1(F); wR(F\textsuperscript{2}) [I &gt; 2σ(I)]</td>
<td>0.0327; 0.0767</td>
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<tr>
<td>R1(F); wR(F\textsuperscript{2}) (all data)</td>
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<td>GoF(F\textsuperscript{2})</td>
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<tr>
<td>Max. residual e\textsuperscript{-} density</td>
<td>0.146 e\textsuperscript{-} \cdot Å\textsuperscript{3}</td>
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