Supplementary Material

One-pot microwave-assisted synthesis of 2,5-bis(pyrazol-4-yl)[1,3]thiazolo[5,4-d][1,3]thiazoles from pyrazole-4-carbaldehydes and dithiooxamide

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$^{13}$C NMR spectrum of compound 2a

$^1$H NMR spectrum of compound 2b
$^{13}$C NMR spectrum of compound 2b

$^1$H NMR spectrum of compound 2c
$^{13}$C NMR spectrum of compound 2c

$^1$H NMR spectrum of compound 2d
X-ray analysis

Crystal data, data collection and structure refinement details are summarized in Table 1.

Table 1 Experimental data and precise structures of compounds 2c

<table>
<thead>
<tr>
<th>Formula</th>
<th>C_{10}H_{13}N_{3}S</th>
</tr>
</thead>
</table>

| Specimen       | colorless plate   |
| Spice dimensions, mm | 0.070 x 0.320 x 0.500 |
| Temperature, K   | 100               |
| Crystal system / Space group | triclinic / P -1 |
| Mr, g/mol        | 207.29            |
| \( \theta_{\text{min}} / \theta_{\text{max}} \) | 2.67/30.25 |
| a, Å; b, Å; c, Å | 5.7032(4); 7.7544(6); 1.9147(8) |
| \( \alpha^\circ; \beta^\circ; \gamma^\circ \) | 89.211(2); 81.328(2); 79.248(3) |
| V, Å^3           | 511.70(6)         |
| Z                | 2                 |
| D_{calc}, g/cm^3 | 1.345             |
| F (000)          | 220               |
| Absorp. Coeff., mm\(^{-1}\) | 0.279 |
| Reflections collected/Independ reflections | 22201 / 3019 |
| Number of ref.param. | 131 |
| Final R₁, % / Rw (all data) | 3.37 / 0.0404 |
| Goodness-of-fit on F^2 | 1.076 |
| \((\Delta \rho)_{\text{max}}\) and \((\Delta \rho)_{\text{min}}, e/Å^3\) | 0.394 and -0.411 |
Weight scheme
\[ w = \frac{1}{\sigma^2(F_o^2) + (0.0419P)^2 + 0.2512P} \]
where \( P = (F_o^2 + 2F_c^2)/3 \)

Principal bond distances, bond angles and torsion angles are presented in Table 2.

**Table 2** Selected bond lengths, bond and torsion angles in compounds 2c

<table>
<thead>
<tr>
<th>( l, \text{Å} )</th>
<th>( \text{Angle} )</th>
<th>( \varphi,^\circ )</th>
<th>( \text{Angle} )</th>
<th>( \theta,^\circ )</th>
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<tbody>
<tr>
<td>1.7296(12)</td>
<td>C6-S1-C5</td>
<td>88.77(5)</td>
<td>C3-N1-N3-C8</td>
<td>1.02(13)</td>
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<tr>
<td>1.3494(14)</td>
<td>C3-N1-C2</td>
<td>127.47(10)</td>
<td>C3-N1-C2-C10</td>
<td>-143.54(12)</td>
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<tr>
<td>1.4718(14)</td>
<td>C5-N2-C6</td>
<td>109.03(10)</td>
<td>C3-N1-C2-C1</td>
<td>92.20(14)</td>
</tr>
<tr>
<td>1.3670(14)</td>
<td>N1-C2-C10</td>
<td>110.20(10)</td>
<td>N3-N1-C3-C4</td>
<td>-0.87(14)</td>
</tr>
<tr>
<td>1.5204(18)</td>
<td>C10-C2-C1</td>
<td>112.39(10)</td>
<td>C6-S1-C5-N2</td>
<td>-0.66(9)</td>
</tr>
<tr>
<td>1.7700(11)</td>
<td>N3-N1-C2</td>
<td>119.09(9)</td>
<td>N1-N3-C8-C4</td>
<td>-0.74(13)</td>
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<td>1.3654(13)</td>
<td>C8-N3-N1</td>
<td>105.11(9)</td>
<td>C3-C4-C5-S1</td>
<td>163.62(10)</td>
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<tr>
<td>1.3201(15)</td>
<td>N1-C2-C1</td>
<td>109.71(10)</td>
<td>C8-C3-C4-O1</td>
<td>179.66(10)</td>
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<td>1.3324(14)</td>
<td>N1-C3-C7</td>
<td>122.81(10)</td>
<td>N1-C3-C4-C5</td>
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<td>1.4907(17)</td>
<td>N2-C5-S1</td>
<td>115.03(8)</td>
<td>C3-C4-C5-N2</td>
<td>-15.86(19)</td>
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<tr>
<td>1.4513(15)</td>
<td>C6-C6-S1</td>
<td>108.92(11)</td>
<td>N3-N1-C2-C10</td>
<td>44.60(14)</td>
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<tr>
<td>1.4008(15)</td>
<td>N3-C8-C9</td>
<td>119.10(10)</td>
<td>N3-N1-C2-C1</td>
<td>-79.66(13)</td>
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