## Supplementary Materials: Molecular Structure, Spectroscopic and DFT Computational Studies of Arylidene-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione

Assem Barakat, Saied M. Soliman, Hazem A. Ghabbour, M. Ali, Abdullah Mohammed Al-Majid, Mohammad Shahidul Islam and Ayman A. Ghfar

Table S1. The calculated bond distances and bond angles compared to the experimental data of 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Calculated</th>
<th>Experimental</th>
<th>Parameter</th>
<th>Calculated</th>
<th>Experimental</th>
</tr>
</thead>
<tbody>
<tr>
<td>R(1-8)</td>
<td>1.228</td>
<td>1.213</td>
<td>A(1-8-6)</td>
<td>117.8</td>
<td>118.6</td>
</tr>
<tr>
<td>R(2-13)</td>
<td>1.221</td>
<td>1.209</td>
<td>A(1-8-19)</td>
<td>125.5</td>
<td>125.2</td>
</tr>
<tr>
<td>R(3-18)</td>
<td>1.225</td>
<td>1.214</td>
<td>A(2-13-6)</td>
<td>121.9</td>
<td>121.2</td>
</tr>
<tr>
<td>R(4-25)</td>
<td>1.361</td>
<td>1.359</td>
<td>A(2-13-7)</td>
<td>122.0</td>
<td>121.5</td>
</tr>
<tr>
<td>R(5-26)</td>
<td>1.364</td>
<td>1.358</td>
<td>A(3-18-7)</td>
<td>119.0</td>
<td>119.9</td>
</tr>
<tr>
<td>R(5-31)</td>
<td>1.425</td>
<td>1.431</td>
<td>A(3-18-19)</td>
<td>123.8</td>
<td>123.3</td>
</tr>
<tr>
<td>R(6-8)</td>
<td>1.401</td>
<td>1.395</td>
<td>A(4-25-23)</td>
<td>120.4</td>
<td>118.2</td>
</tr>
<tr>
<td>R(6-9)</td>
<td>1.469</td>
<td>1.465</td>
<td>A(4-25-26)</td>
<td>120.3</td>
<td>121.8</td>
</tr>
<tr>
<td>R(6-13)</td>
<td>1.397</td>
<td>1.375</td>
<td>A(26-5-31)</td>
<td>118.7</td>
<td>118.0</td>
</tr>
<tr>
<td>R(7-13)</td>
<td>1.395</td>
<td>1.365</td>
<td>A(5-26-25)</td>
<td>113.7</td>
<td>115.4</td>
</tr>
<tr>
<td>R(7-14)</td>
<td>1.468</td>
<td>1.477</td>
<td>A(5-26-27)</td>
<td>126.2</td>
<td>124.6</td>
</tr>
<tr>
<td>R(7-18)</td>
<td>1.395</td>
<td>1.389</td>
<td>A(8-6-9)</td>
<td>116.2</td>
<td>117.5</td>
</tr>
<tr>
<td>R(8-19)</td>
<td>1.471</td>
<td>1.475</td>
<td>A(8-6-13)</td>
<td>126.0</td>
<td>125.7</td>
</tr>
<tr>
<td>R(18-19)</td>
<td>1.491</td>
<td>1.485</td>
<td>A(6-8-19)</td>
<td>116.6</td>
<td>116.2</td>
</tr>
<tr>
<td>R(19-20)</td>
<td>1.373</td>
<td>1.357</td>
<td>A(9-6-13)</td>
<td>117.7</td>
<td>116.8</td>
</tr>
<tr>
<td>R(20-22)</td>
<td>1.448</td>
<td>1.455</td>
<td>A(6-13-7)</td>
<td>116.1</td>
<td>117.3</td>
</tr>
<tr>
<td>R(22-23)</td>
<td>1.421</td>
<td>1.413</td>
<td>A(13-7-14)</td>
<td>118.1</td>
<td>116.9</td>
</tr>
<tr>
<td>R(22-29)</td>
<td>1.411</td>
<td>1.384</td>
<td>A(13-7-18)</td>
<td>125.3</td>
<td>125.4</td>
</tr>
<tr>
<td>R(23-25)</td>
<td>1.382</td>
<td>1.368</td>
<td>A(14-7-18)</td>
<td>116.6</td>
<td>117.7</td>
</tr>
<tr>
<td>R(25-26)</td>
<td>1.413</td>
<td>1.383</td>
<td>A(7-18-19)</td>
<td>117.2</td>
<td>116.8</td>
</tr>
<tr>
<td>R(26-27)</td>
<td>1.395</td>
<td>1.384</td>
<td>A(8-19-18)</td>
<td>118.7</td>
<td>118.4</td>
</tr>
<tr>
<td>R(27-29)</td>
<td>1.392</td>
<td>1.411</td>
<td>A(8-19-20)</td>
<td>127.7</td>
<td>127.4</td>
</tr>
<tr>
<td>A(18-19-20)</td>
<td>113.6</td>
<td>114.2</td>
<td>A(19-20-22)</td>
<td>138.6</td>
<td>137.8</td>
</tr>
<tr>
<td>A(20-22-23)</td>
<td>114.8</td>
<td>114.2</td>
<td>A(20-22-29)</td>
<td>127.2</td>
<td>127.9</td>
</tr>
<tr>
<td>A(23-22-29)</td>
<td>118.1</td>
<td>117.8</td>
<td>A(22-23-25)</td>
<td>121.5</td>
<td>121.7</td>
</tr>
<tr>
<td>A(22-29-27)</td>
<td>120.6</td>
<td>120.6</td>
<td>A(23-25-26)</td>
<td>119.3</td>
<td>120.0</td>
</tr>
<tr>
<td>A(25-26-27)</td>
<td>120.1</td>
<td>120.1</td>
<td>A(26-27-29)</td>
<td>120.4</td>
<td>119.8</td>
</tr>
</tbody>
</table>
Table S2. The calculated bond distances and bond angles compared to the experimental data of 2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Calculated</th>
<th>Experimental</th>
<th>Parameter</th>
<th>Calculated</th>
<th>Experimental</th>
</tr>
</thead>
<tbody>
<tr>
<td>R(1-8)</td>
<td>1.226</td>
<td>1.218</td>
<td>A(1-8-6)</td>
<td>120.1</td>
<td>119.4</td>
</tr>
<tr>
<td>R(2-13)</td>
<td>1.22</td>
<td>1.224</td>
<td>A(1-8-19)</td>
<td>123.3</td>
<td>123.7</td>
</tr>
<tr>
<td>R(3-18)</td>
<td>1.229</td>
<td>1.213</td>
<td>A(2-13-6)</td>
<td>121.5</td>
<td>120.5</td>
</tr>
<tr>
<td>R(4-25)</td>
<td>1.359</td>
<td>1.363</td>
<td>A(2-13-7)</td>
<td>121.3</td>
<td>121.4</td>
</tr>
<tr>
<td>R(4-31)</td>
<td>1.423</td>
<td>1.433</td>
<td>A(3-18-7)</td>
<td>118.9</td>
<td>118.0</td>
</tr>
<tr>
<td>R(5-26)</td>
<td>1.354</td>
<td>1.346</td>
<td>A(3-18-19)</td>
<td>124.9</td>
<td>124.9</td>
</tr>
<tr>
<td>R(6-8)</td>
<td>1.397</td>
<td>1.381</td>
<td>A(25-4-31)</td>
<td>117.6</td>
<td>117.4</td>
</tr>
<tr>
<td>R(6-9)</td>
<td>1.468</td>
<td>1.471</td>
<td>A(4-25-23)</td>
<td>125.0</td>
<td>125.2</td>
</tr>
<tr>
<td>R(6-13)</td>
<td>1.391</td>
<td>1.367</td>
<td>A(4-25-26)</td>
<td>115.2</td>
<td>114.3</td>
</tr>
<tr>
<td>R(7-13)</td>
<td>1.394</td>
<td>1.373</td>
<td>A(5-26-25)</td>
<td>117.1</td>
<td>117.4</td>
</tr>
<tr>
<td>R(7-14)</td>
<td>1.468</td>
<td>1.465</td>
<td>A(5-26-27)</td>
<td>123.3</td>
<td>123.3</td>
</tr>
<tr>
<td>R(7-18)</td>
<td>1.403</td>
<td>1.399</td>
<td>A(8-6-9)</td>
<td>119.3</td>
<td>118.1</td>
</tr>
<tr>
<td>R(8-19)</td>
<td>1.493</td>
<td>1.482</td>
<td>A(8-6-13)</td>
<td>124.9</td>
<td>124.7</td>
</tr>
<tr>
<td>R(18-19)</td>
<td>1.472</td>
<td>1.455</td>
<td>A(6-8-19)</td>
<td>116.7</td>
<td>116.9</td>
</tr>
<tr>
<td>R(19-20)</td>
<td>1.376</td>
<td>1.367</td>
<td>A(9-6-13)</td>
<td>115.9</td>
<td>117.2</td>
</tr>
<tr>
<td>R(20-22)</td>
<td>1.445</td>
<td>1.439</td>
<td>A(6-13-7)</td>
<td>117.2</td>
<td>118.2</td>
</tr>
<tr>
<td>R(22-23)</td>
<td>1.419</td>
<td>1.405</td>
<td>A(13-7-14)</td>
<td>115.3</td>
<td>117.6</td>
</tr>
<tr>
<td>R(22-29)</td>
<td>1.413</td>
<td>1.403</td>
<td>A(13-7-18)</td>
<td>125.6</td>
<td>124.3</td>
</tr>
<tr>
<td>R(23-25)</td>
<td>1.386</td>
<td>1.37</td>
<td>A(14-7-18)</td>
<td>119.1</td>
<td>118.1</td>
</tr>
<tr>
<td>R(25-26)</td>
<td>1.419</td>
<td>1.403</td>
<td>A(7-18-19)</td>
<td>116.2</td>
<td>117.1</td>
</tr>
<tr>
<td>R(26-27)</td>
<td>1.396</td>
<td>1.38</td>
<td>A(8-19-18)</td>
<td>119.6</td>
<td>118.6</td>
</tr>
<tr>
<td>R(27-29)</td>
<td>1.388</td>
<td>1.372</td>
<td>A(8-19-20)</td>
<td>113.2</td>
<td>114.0</td>
</tr>
</tbody>
</table>

© 2016 by the authors; licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons by Attribution (CC-BY) license (http://creativecommons.org/licenses/by/4.0/).