The crystal structure of 2-chloro-4-(prop-2-yn-1-yloxy)-6-phenyl-1,3,5-triazine, C_{12}H_8ClN_3O

Table 1: Data collection and handling.

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>U_{iso}/*U_{eq}</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>0.66930(7)</td>
<td>0.67265(17)</td>
<td>0.63980(7)</td>
<td>0.0301(3)</td>
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<tr>
<td>C2</td>
<td>0.72000(6)</td>
<td>0.56251(15)</td>
<td>0.55580(7)</td>
<td>0.0249(3)</td>
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<tr>
<td>C3</td>
<td>0.59710(6)</td>
<td>0.62754(16)</td>
<td>0.51169(7)</td>
<td>0.0251(3)</td>
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<tr>
<td>C4</td>
<td>0.78541(7)</td>
<td>0.49855(15)</td>
<td>0.53929(8)</td>
<td>0.0278(3)</td>
</tr>
<tr>
<td>C5</td>
<td>0.85612(7)</td>
<td>0.48345(18)</td>
<td>0.60218(9)</td>
<td>0.0352(3)</td>
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<tr>
<td>H5</td>
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<td>0.042*</td>
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<tr>
<td>H6</td>
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<td>0.4178</td>
<td>0.6280</td>
<td>0.052*</td>
</tr>
<tr>
<td>C7</td>
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<td>0.50665(11)</td>
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<tr>
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<tr>
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</table>

Source of material

Under the protection of N_2, Mg (3.84 g, 0.160 mol) and I_2 (1.02 g, 0.004 mol) were added to the solution of tetrahydrofuran (150 mL). After 10 mins bromobenzene (25 g, 0.160 mol) was added to the suspension mixture dropwisely. When the solid Mg disappeared, the reaction mixture was cooled to −15 °C. A solution of 2,4,6-trichloro-1,3,5-triazine (31.75 g, 0.175 mol) in tetrahydrofuran was added to the above solution of PhMgBr in 5 min. After 2 h, the mixture was filtered and...
the filtrate was evaporated to get a yellow solid, which was purified by chromatography on silica gel to get the 2,4-dichloro-6-phenyl-1,3,5-triazine (27.85 g, yield 77%) as a white solid. To a suspension of 2,4-dichloro-6-phenyl-1,3,5-triazine (2.26 g, 0.01 mol) in 60 mL of tetrahydrofuran was added K$_2$CO$_3$ (2.76 g, 0.02 mol) and propiolic alcohol (0.62 g, 0.011 mol). The mixture was refluxed for 6 h and then filtered to get a yellow solution. The solvent was evaporated under reduced pressure to get a yellow solid which was purified by chromatography on silica gel to afford 2-chloro-4-(prop-2-yn-1-yloxy)-6-phenyl-1,3,5-triazine as a white solid. (1.55 g, 63%).

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References