The title compound, C$_{16}$H$_{12}$Cl$_2$OS, crystallizes in a non-centrosymmetric space group and shows a significant nonlinear optical activity. The source of the optical activity lies in the twist of the chalcone backbone, as exemplified by the dihedral angle of 42.45 (6)$^\circ$ between the two benzene rings. Weak intermolecular C–H···O hydrogen bonds may contribute to the stabilization of the crystal structure.

Comment

A non-centrosymmetric crystal packing of molecules is a prerequisite for second-order nonlinear optical (NLO) activity, and much attention has been focused on this aspect of molecular structure (Long, 1995) and organic NLO materials due to their promising applications in optoelectronics technology and the much larger nonlinear response, extremely fast switching time and convenient optimization routes through molecular engineering compared with the currently studied inorganic materials. To have strong second-order NLO properties, the compound must possess a large first-order molecular hyperpolarizability, $\beta$, and also must crystallize in a non-centrosymmetric structure to have a non-zero $\chi^2$. Besides the strong NLO properties, the materials must also fulfill some other requirements such as good transparency and high thermal stability (Zhao et al., 2000).
methoxyphenyl)prop-2-en-1-one and 1-(4-bromophenyl)-3-(2,4-dichlorophenyl)prop-2-en-1-one have been reported (Patil, Ng et al., 2006; Patil, Rosli et al., 2006; Patil, Teh et al., 2006). In continuation of our quest to synthesize new chalcones (Butcher, Yathirajan, Sarojini et al., 2006; Butcher et al., 2006a,b), we have synthesized a new chalcone and studied its SHG efficiency. In view of the importance of the title compound, (I), its crystal structure is reported here.

The structure of (I) shows similar metrical parameters to those observed in other structurally characterized chalcones (Patil, Ng et al., 2006; Patil, Rosli et al., 2006; Patil, Teh et al., 2006; Butcher, Yathirajan, Sarojini et al., 2006; Butcher et al., 2006a,b). Since these molecules do not possess a chiral center, the source of the optical activity lies in the twist of the chalcone backbone. This is best exemplified by the dihedral angle of 42.45 (6)°, between the planes of the two phenyl rings. There is a weak hydrogen bond between one of the methyl H atoms and the C=O group of an adjoining molecule (Table 2).

### Experimental

To a mixture of 4-methylthiobenzaldehyde (1.52 g, 0.01 mol) and 2,4-dichloroacetophenone (1.89 g, 0.01 mol) in ethanol (5 ml), an aqueous solution of potassium hydroxide (5%, 5 ml) was added slowly with stirring. The mixture was stirred at room temperature for 24 h. The precipitated solid was filtered off, washed with water, dried and recrystallized from acetone (yield 70%; m.p. 384 K; SHG 0.44 mm). The purity of the product was tested using an Nd:YAG laser.

### Crystal data

\begin{align*}
\text{C}_{16}\text{H}_{12}\text{Cl}_{2}\text{O}_{2} & , Z = 2 \\
M_r & = 323.22 \\
\text{Monoclinic, P2}_1 & \text{ Å} \\
\alpha & = 12.957 (3) \text{ Å} \\
b & = 3.8920 (8) \text{ Å} \\
c & = 14.135 (3) \text{ Å} \\
\beta & = 97.736 (2) \text{°} \\
V & = 706.3 (3) \text{ Å}^3
\end{align*}

### Data collection

- **Bruker APEX-II CCD area-detector diffractometer**
- **\(\varphi\) and \(\omega\) scans**
- **Absorption correction: multi-scan (SADABS; Sheldrick, 1996)**
- **\(T_{\text{max}}\) = 0.712, \(T_{\text{min}}\) = 0.937**
- **6061 measured reflections**
- **2993 independent reflections**
- **2893 reflections with \(I > 2\sigma(I)\)**
- **\(R_{\text{int}}\) = 0.021**
- **\(\theta_{\text{max}}\) = 28.1°**

### Refinement

- **crystal size**: \(a = 0.35 \times 0.25 \times 0.25 \text{ mm}^3\)
- **maximal Flack parameter**: 0.16 (6)
- **min R-factor (I)**
- **Displacement ellipsoids are drawn at the 50% probability level.**

### Table 1

Selected geometric parameters (\(\text{Å}, \text{°}\)).

<table>
<thead>
<tr>
<th>Bond</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>C11–C12</td>
<td>1.7430 (19)</td>
</tr>
<tr>
<td>C12–C13</td>
<td>1.7411 (19)</td>
</tr>
<tr>
<td>C13–C14</td>
<td>1.7564 (18)</td>
</tr>
<tr>
<td>C14–C16</td>
<td>1.801 (2)</td>
</tr>
<tr>
<td>O–C7</td>
<td>1.227 (2)</td>
</tr>
<tr>
<td>C7–C8</td>
<td>1.473 (2)</td>
</tr>
<tr>
<td>C8–C9</td>
<td>1.343 (3)</td>
</tr>
<tr>
<td>C9–C10</td>
<td>1.345 (3)</td>
</tr>
<tr>
<td>C10–C11</td>
<td>1.339 (3)</td>
</tr>
<tr>
<td>C11–C12</td>
<td>1.276 (2)</td>
</tr>
<tr>
<td>C12–C13</td>
<td>1.241 (2)</td>
</tr>
<tr>
<td>C13–C14</td>
<td>1.238 (2)</td>
</tr>
<tr>
<td>C14–C15</td>
<td>1.250 (2)</td>
</tr>
<tr>
<td>C15–C16</td>
<td>1.250 (2)</td>
</tr>
<tr>
<td>C16–O</td>
<td>1.239 (2)</td>
</tr>
<tr>
<td>C16–H16</td>
<td>0.98 3.21 3.852 (3) 125</td>
</tr>
</tbody>
</table>

### Table 2

Hydrogen-bond geometry (\(\text{Å}, \text{°}\)).

<table>
<thead>
<tr>
<th>Bond</th>
<th>D–H⋯A</th>
<th>D–H</th>
<th>H⋯A</th>
<th>D⋯A</th>
<th>D–H⋯A</th>
</tr>
</thead>
<tbody>
<tr>
<td>C16–H16B⋯O1</td>
<td>0.98</td>
<td>3.21</td>
<td>3.852 (3)</td>
<td>125</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry code: (i) \(-x+1, y+\frac{1}{2}, -z+2\). H atoms were positioned geometrically, with C–H = 0.95 and methyl H, respectively, and constrained to ride on their parent atoms, with \(U_{eq}(H) = xU_{eq}(C)\), where \(x = 1.5\) for methyl H and \(x = 1.2\) for all other H atoms. The value of the Flack parameter suggests possible partial inversion twinning.

Data collection: SMART (Bruker, 2006); cell refinement: SAINT (Bruker, 2006); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2003); software used to prepare material for publication: SHELXTL.

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**Figure 1**
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

**Figure 2**
A packing diagram of (I).
References


