

2,2-Dichloro-1-(4-ethoxyphenyl)cyclopropanyl  
piperidin-1-yl ketoneNa-Bo Sun,<sup>a</sup> De-Long Shen,<sup>a\*</sup>  
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## Key indicators

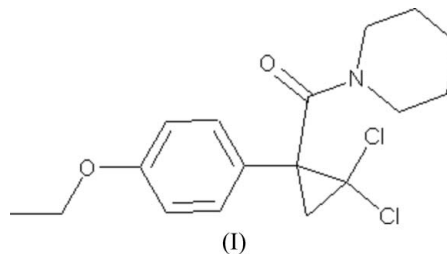
Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.035  
 $wR$  factor = 0.081  
Data-to-parameter ratio = 19.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The title compound,  $\text{C}_{17}\text{H}_{21}\text{Cl}_2\text{NO}_2$ , a cyclopropane derivative related to the insecticide cycloprothrin, was prepared from piperidine and 2,2-dichloro-1-(4-ethoxyphenyl)cyclopropanecarbonyl chloride. The six-membered piperidine ring has a chair conformation. The orientation of the carbonyl group relative to the cyclopropane ring may be described by the torsion angle  $X-\text{C}-\text{C}=\text{O}$  of  $-98.3^\circ$ , where  $X$  is the centroid of the cyclopropane ring.

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## Comment

Cycloprothrin derivatives have a high potential for biological activity; they are commonly characterized by low toxicity and good environmental compatibility. These derivatives have been widely used in the manufacture of pesticides (Holan *et al.*, 1986). As part of our ongoing studies of structure–activity relationships for cycloprothrin derivatives and related compounds, we have isolated the title compound, (I), by the reaction of piperidine and 2,2-dichloro-1-(4-ethoxyphenyl)-cyclopropanecarbonyl chloride.



The molecular structure of (I) is shown in Fig. 1. Atoms C5, C6, C8 and C9 are coplanar within 0.0284 Å, and the C5–C9/N1 ring has a chair conformation (Cremer & Pople, 1975). The C2–C1–C4–O1 torsion angle is  $-65.82(17)^\circ$  and C3–C1–C4–O1 is  $-133.21(14)^\circ$ . The orientation of the carbonyl group relative to the cyclopropane ring may be described by the torsion angle  $X-\text{C1}-\text{C4}-\text{O1}$  of  $-98.3^\circ$ , where  $X$  is the centroid of the cyclopropane ring.

## Experimental

Piperidine (0.75 g, 8.8 mmol) and triethylamine (1.2 g, 11.9 mmol) were dissolved in dichloromethane (15 ml) with stirring, and 2,2-dichloro-1-(4-ethoxyphenyl)cyclopropanecarbonyl chloride (2.75 g, 10 mmol) was added dropwise to the mixture at room temperature. The mixture was then stirred at room temperature for 15 h, washed three times with water and dried, yielding 2.77 g of a solid product (yield 92.0%). This was recrystallized from ethanol and gave colourless chunks (m.p. 394–396 K) suitable for an X-ray crystallographic study.

## Crystal data

$C_{17}H_{21}Cl_2NO_2$   
 $M_r = 342.26$   
 Monoclinic,  $P2_1/n$   
 $a = 6.0819$  (19) Å  
 $b = 15.592$  (6) Å  
 $c = 18.000$  (7) Å  
 $\beta = 91.087$  (14)°  
 $V = 1706.6$  (10) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.332$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.39$  mm<sup>-1</sup>  
 $T = 296$  (1) K  
 Chunk, colourless  
 $0.40 \times 0.38 \times 0.30$  mm

## Data collection

Rigaku R-Axis RAPID  
 diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.846$ ,  $T_{\max} = 0.891$

16067 measured reflections  
 3899 independent reflections  
 2653 reflections with  $F^2 > 2\sigma(F^2)$   
 $R_{\text{int}} = 0.033$   
 $\theta_{\text{max}} = 27.5^\circ$

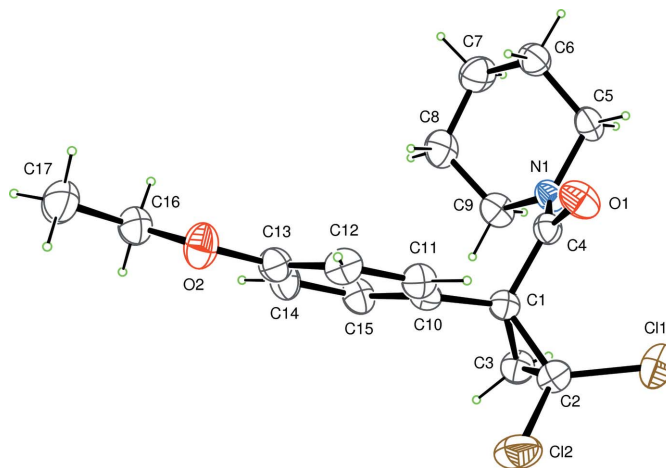
## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.081$   
 $S = 1.00$   
 3899 reflections  
 200 parameters  
 H-atom parameters constrained

$w = 1/[0.0002F_o^2 + 1.1\sigma(F_o^2)]/(4F_o^2)$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.40$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.38$  e Å<sup>-3</sup>  
 Extinction correction: Larson  
 (1970), equation 22  
 Extinction coefficient: 99 (19)

H atoms were included in calculated positions and refined using a riding model. H atoms were given isotropic displacement parameters equal to 1.2 (or 1.5 for methyl H atoms) times  $U_{\text{eq}}$  of their parent atoms and C—H distances were restrained to 0.96 Å for methyl H atoms, 0.93 Å for aromatic H atoms and 0.97 Å for the remainder.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1993); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.



**Figure 1**

The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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