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## Key indicators

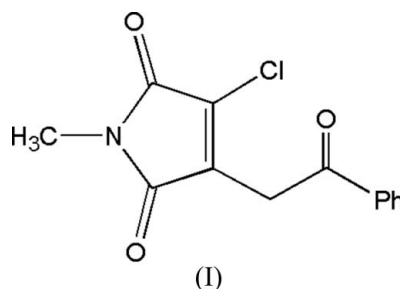
Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.049  
 $wR$  factor = 0.150  
Data-to-parameter ratio = 12.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.3-Benzoylmethyl-2-chloro-*N*-methylmaleimide

In the title compound,  $\text{C}_{13}\text{H}_{10}\text{ClNO}_3$ , the dihedral angle between the two rings is  $68.9(3)^\circ$ . The crystal structure is stabilized by weak intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds.

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## Comment

We have investigated the photo-induced reaction of 3,4-dichloromaleimide (3,4-dichloro-pyrrole-2,5-dione) and 2-trimethylsilyloxyphenylethene, and obtained the title compound, (I), as one of the products. An X-ray crystallographic analysis was undertaken to establish its structure and configuration.



In the structure of (I) (Fig. 1), bond lengths and angles are in good agreement with the expected values (Allen *et al.*, 1987). Both the maleimide ring and the phenyl ring are planar to within  $\pm 0.02$  Å. The carbonyl group linked to the phenyl ring is nearly in the plane of the phenyl ring, with atom C7 deviating by  $0.019(3)$  Å. Similarly, atom Cl1 is in the plane of the maleimide ring, with a deviation of  $0.045(3)$  Å. The deviations of atom C8 from the phenyl and maleimide rings are  $0.058(2)$  and  $0.100(2)$  Å, respectively. Finally, the dihedral angle between the phenyl and maleimide rings is  $68.9(3)^\circ$ .

In the packing of the title compound, the molecules are linked into layers (Fig. 2) by  $\text{C}-\text{H}\cdots\text{O}$  intermolecular contacts (Table 2). No significant  $\pi-\pi$  interactions are observed in the crystal structure.

## Experimental

The title compound was one of the products of a photo-induced reaction between 3,4-dichloromaleimide ( $0.5 \text{ mol l}^{-1}$ ) (3,4-dichloro-pyrrole-2,5-dione) and an excess amount of 2-trimethylsilyloxyphenylethene ( $1.5 \text{ mol l}^{-1}$ ) in benzene. The solution was irradiated for 10 h with UV light of  $\lambda > 300$  nm. The title compound was isolated using column chromatography (yield 35%). Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a petroleum ether–ethyl acetate (4:1) solution.

## Crystal data

$C_{13}H_{10}ClNO_3$   
 $M_r = 263.67$   
 Monoclinic,  $P2_1/n$   
 $a = 5.474$  (2) Å  
 $b = 24.185$  (3) Å  
 $c = 9.283$  (2) Å  
 $\beta = 98.78$  (3)°  
 $V = 1214.4$  (5) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.442$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 25 reflections  
 $\theta = 1.7$ – $25.0$ °  
 $\mu = 0.31$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 Plate, colourless  
 $0.40 \times 0.40 \times 0.10$  mm

## Data collection

Enraf–Nonius CAD-4 diffractometer  
 $\omega/2\theta$  scans  
 Absorption correction:  $\psi$  scan (XCAD4; Harms & Wocadlo, 1995)  
 $T_{\min} = 0.885$ ,  $T_{\max} = 0.965$   
 2298 measured reflections  
 2085 independent reflections

1321 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.066$   
 $\theta_{\text{max}} = 25.0$ °  
 $h = 0 \rightarrow 6$   
 $k = 0 \rightarrow 28$   
 $l = -11 \rightarrow 10$   
 3 standard reflections every 200 reflections  
 intensity decay: none

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.049$   
 $wR(F^2) = 0.150$   
 $S = 1.03$   
 2085 reflections  
 163 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.003$   
 $\Delta\rho_{\text{max}} = 0.32$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>  
 Extinction correction: *SHELXTL* (Sheldrick, 1997)  
 Extinction coefficient: 0.022 (3)

Table 1

Selected geometric parameters (Å, °).

O1–C7	1.211 (3)	C7–C8	1.516 (4)
C5–C7	1.481 (4)	C12–Cl	1.700 (3)
C5–C7–C8	118.5 (3)	C11–C12–Cl	120.4 (2)
C9–C8–C7	112.6 (3)	C7–C8–C9–C10	–68.3 (4)
C6–C5–C7–C8	3.5 (4)	N–C11–C12–Cl	–179.2 (2)
C5–C7–C8–C9	169.7 (3)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3–H3A $\cdots$ O3 <sup>i</sup>	0.93	2.59	3.499 (5)	163
C8–H8B $\cdots$ O1 <sup>ii</sup>	0.97	2.51	3.375 (5)	147

Symmetry codes: (i)  $-x - \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (ii)  $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ .

H atoms were positioned geometrically and treated as riding on their parent C atoms, with C–H distances constrained to 0.93 (aromatic CH), 0.97 (methylene CH<sub>2</sub>) or 0.96 Å (methyl CH<sub>3</sub>), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic CH and methylene CH<sub>2</sub>, or  $1.5U_{\text{eq}}(\text{C})$  for the methyl group.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*;

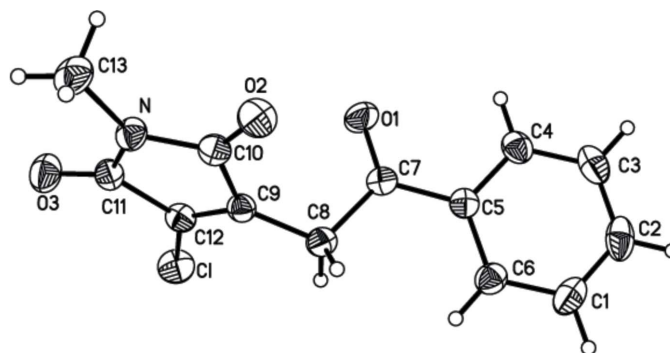


Figure 1

The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

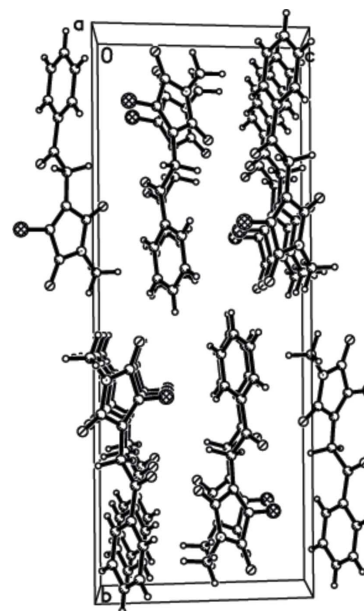


Figure 2

The crystal structure of (I), viewed along [100].

molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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## References

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