

## Yong Sun

Yunyang Teachers College, Danjiangkou  
442700, People's Republic of China

Correspondence e-mail: suny6135@126.com

## Key indicators

Single-crystal X-ray study  
 $T = 292$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.049  
 $wR$  factor = 0.134  
Data-to-parameter ratio = 17.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.4-(4-Methoxybenzylidene)-2-(4-morpholino)-  
1-phenyl-1*H*-imidazol-5(4*H*)-one

In the title compound,  $\text{C}_{21}\text{H}_{21}\text{N}_3\text{O}_3$ , the five-membered imidazolone ring is planar. The packing of the molecules in the crystal structure is mainly due to intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen-bonding interactions.

Received 30 October 2006  
Accepted 8 November 2006

## Comment

Imidazolinones are important heterocycles which exhibit good biological and pharmaceutical activities (Solankee *et al.*, 2001). Recently, many derivatives of imidazolinone have been prepared and their biological activities studied (Ding *et al.*, 2005). As part of our work on the preparation of potentially active heterocycles, we report here the crystal structure of the title compound, (I).

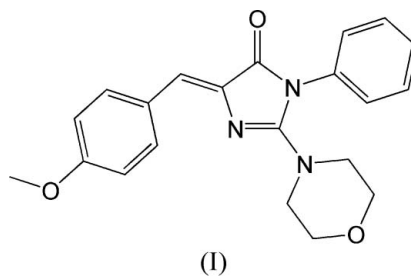


Fig. 1 show the molecular structure of (I), with the atomic numbering scheme. The five-membered imidazolinone ring in (I) is planar. The benzene ring is twisted with respect to this imidazolinone ring, with a  $\text{C}12-\text{C}11-\text{N}1-\text{C}10$  torsion angle of  $67.11(16)^\circ$ . The  $\text{C}7-\text{C}8-\text{C}9-\text{N}2$  torsion angle of  $-2.0(2)^\circ$  indicates a *Z* configuration of the molecule about the  $\text{C}8=\text{C}9$  bond. There are intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen-bonding interactions (Fig. 2).

## Experimental

To a solution of *N*-[1-ethoxycarbonyl-2-(4-methoxyphenyl)ethen-1-yl]iminophosphorane (1.44 g, 3 mmol) in dry dichloromethane (15 ml) was added phenyl isocyanate (0.36 g, 3 mmol) under nitrogen at room temperature. After the reaction mixture had been allowed to stand for 6 h at room temperature, the solvent was removed under reduced pressure and diethyl ether–petroleum ether (1:2, 20 ml) was added to precipitate the triphenylphosphine oxide. After filtration, the solvent was removed to give the carbodiimide, which was used directly without further purification. To a solution of the carbodiimide, prepared as above, in dichloromethane (15 ml) was added morpholine (0.26 g, 3 mmol). After the reaction mixture had been allowed to stand for 6 h, the solution was concentrated under reduced pressure and the residue was recrystallized from dichloromethane–petroleum ether (1:4) to give the title compound (I) in a yield of 91%

(m.p. 495 K). Suitable crystals of (I) were obtained by vapour diffusion of ethanol into a dichloromethane solution at room temperature.

#### Crystal data

$C_{21}H_{21}N_3O_3$	$V = 927.76 (18) \text{ \AA}^3$
$M_r = 363.41$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.301 \text{ Mg m}^{-3}$
$a = 7.6366 (9) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.6475 (12) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 12.8267 (14) \text{ \AA}$	$T = 292 (2) \text{ K}$
$\alpha = 69.167 (2)^\circ$	Block, colourless
$\beta = 76.885 (2)^\circ$	$0.40 \times 0.30 \times 0.20 \text{ mm}$
$\gamma = 74.118 (2)^\circ$	

#### Data collection

Bruker SMART CCD area-detector diffractometer	4200 independent reflections
$\varphi$ and $\omega$ scans	3378 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.063$
10789 measured reflections	$\theta_{\text{max}} = 27.5^\circ$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 0.0643P]$
$R[F^2 > 2\sigma(F^2)] = 0.049$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.134$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
4200 reflections	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
245 parameters	
H-atom parameters constrained	

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C16-H16\cdots O1^i$	0.93	2.52	3.3843 (19)	156
$C8-H8\cdots O2^{ii}$	0.93	2.41	3.3151 (16)	165
$C18-H18B\cdots N1$	0.97	2.61	2.9596 (16)	102
$C5-H5\cdots N2$	0.93	2.48	3.1072 (18)	125
$C4-H4\cdots O3^{iii}$	0.93	2.47	3.3225 (17)	153

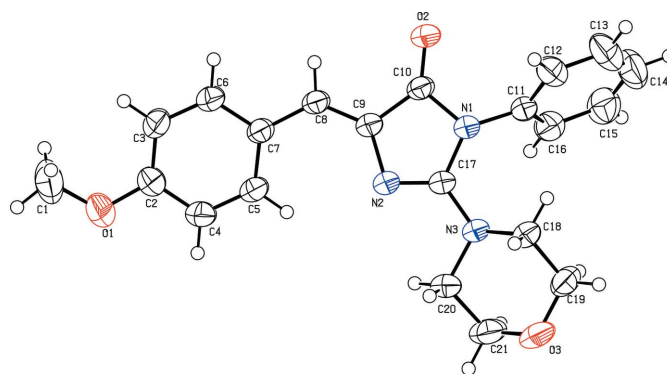
Symmetry codes: (i)  $-x+1, -y, -z+1$ ; (ii)  $-x, -y+1, -z+1$ ; (iii)  $-x+2, -y, -z+1$ .

H atoms were placed at calculated positions and treated as riding atoms [ $C-H = 0.93$  (CH),  $0.97$  ( $\text{CH}_2$ ) and  $0.96 \text{ \AA}$  ( $\text{CH}_3$ )],  $U_{\text{iso}}(\text{H}) = 1.2$  (CH and  $\text{CH}_2$ ) or  $1.5$  ( $\text{CH}_3$ ) times  $U_{\text{eq}}(\text{C})$ .

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

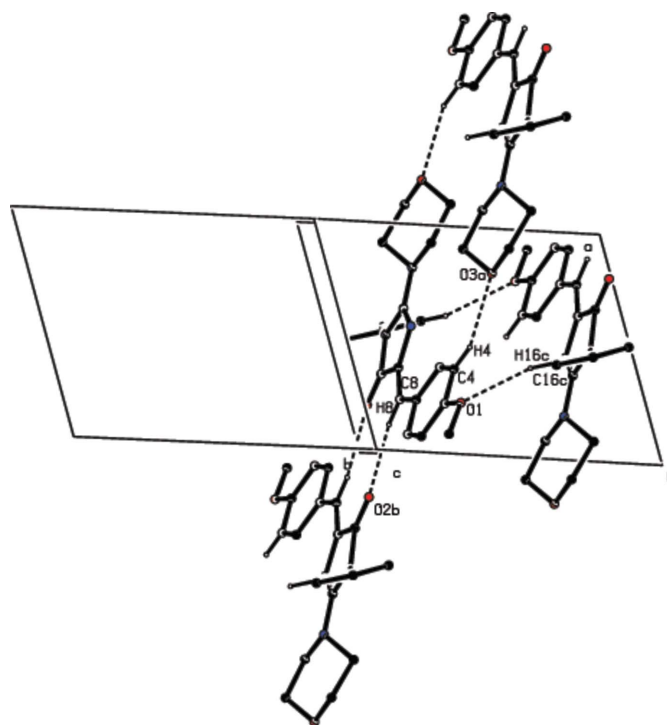
#### References

- Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Ding, M. W., Fu, B. Q. & Yuan, J. Z. (2005). *Heteroat. Chem.* **16**, 76–80.



**Figure 1**

The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.



**Figure 2**

Packing diagram of (I), showing hydrogen-bonding interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted.

- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.  
Solankee, A., Kapadia, K., Upadhyay, K. & Patel, J. (2001). *Orient. J. Chem.* **17**, 315–318.