

C11—N10—C15	108.1 (2)	C14—O13—C12	109.3 (2)
C11—N10—C9	112.2 (2)	O13—C14—C15	112.5 (3)
C15—N10—C9	109.3 (2)	N10—C15—C14	110.6 (2)
N10—C11—C12	109.6 (2)	N17—C18—C18 <sup>b</sup>	109.7 (2)
O13—C12—C11	110.4 (3)		
C15—N10—C11—C12	-59.1 (3)	C11—N10—C15—C14	55.9 (3)
N10—C11—C12—O13	62.1 (3)	O13—C14—C15—N10	-56.2 (3)
C11—C12—O13—C14	-59.6 (3)	C16—N17—C18—C18 <sup>b</sup>	130.4 (3)
C12—O13—C14—C15	57.0 (3)		

Symmetry code: (i)  $1 - x, 1 - y, 1 - z$ .

Table 4. Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ) for (II)

D—H...A	D—H	H...A	D...A	D—H...A
O7—H7...N17	0.94 (4)	1.69 (4)	2.577 (3)	156 (3)

Each data collection covered a hemisphere of reciprocal space by a combination of three sets of exposures; each set had a different  $\varphi$  angle (0, 88 and  $180^\circ$ ) for the crystal and each exposure of 30 s covered  $0.3^\circ$  in  $\omega$ . The crystal-to-detector distance was 4 cm and the detector swing angle was  $-35^\circ$ . Coverage of the unique set is over 99% complete. Crystal decay was monitored by repeating thirty initial frames at the end of data collection and analysing the duplicate reflections, and was found to be negligible.

The structures were solved by direct methods and refined by full-matrix least-squares techniques. All the H atoms were geometrically fixed and allowed to ride on the parent C atoms except the phenyloxy-H atom (H7) which was located from the difference Fourier map and refined isotropically in both the compounds.

For both compounds, data collection: *SMART* (Siemens, 1996a); cell refinement: *SAINT* (Siemens, 1996b); data reduction: *SAINT*; program(s) used to solve structures: *SHELXTL* (Sheldrick, 1996); program(s) used to refine structures: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PARST* (Nardelli, 1995).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: HA1231). Services for accessing these data are described at the back of the journal.

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## 5-Benzoyl-1-ethyl-4-phenyl-1H-pyrimidin-2-one

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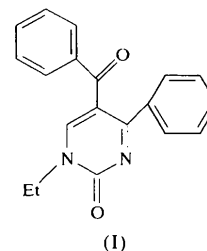
## Abstract

In the title compound,  $\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}_2$ , the pyrimidine ring is distorted from planarity. The dihedral angle between the two phenyl rings is  $88.3(1)^\circ$ . The two phenyl rings form dihedral angles of  $114.6(1)$  and  $141.2(1)^\circ$  with the pyrimidine ring.

## Comment

Pyrimidines in general are of great biological and medicinal interest and for this reason their chemistry has been extensively investigated (Brown, 1984, 1985). In particular, various analogues of thiopyrimidines possess effective antibacterial, antifungal, antiviral, insecticidal and mitocidal activity (Sankyo Co., 1984; Akçamur *et al.*, 1988; Özbey *et al.*, 1991; Akkurt *et al.*, 1992; Akkurt & Hiller, 1993).

The bond lengths and bond angles observed in the title structure, (I), show normal values (Öztürk *et al.*, 1997). The pyrimidine ring is distorted from



planarity with a maximum deviation of  $0.095(4) \text{\AA}$  for C2. The dihedral angle between the two phenyl rings is  $88.3(1)^\circ$  and they form dihedral angles of  $114.6(1)$  and  $141.2(1)^\circ$  with the pyrimidine ring. The shortest intermolecular contact observed in the structure is  $3.209(5) \text{\AA}$  between C1 and O1( $x, \frac{1}{2} - y, z - \frac{1}{2}$ ). The crystal structure is stabilized by van der Waals contacts.

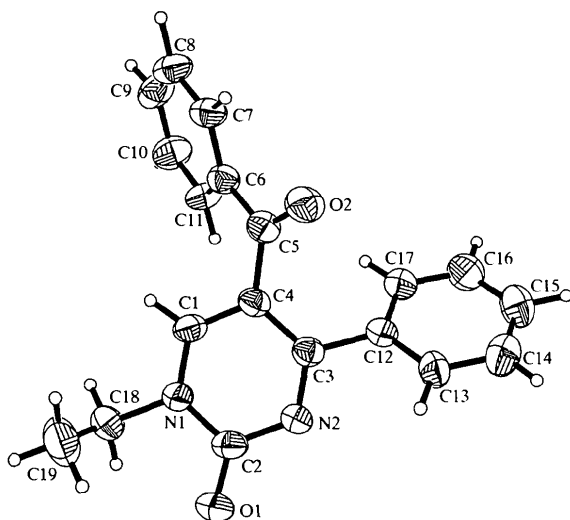


Fig. 1. The structure of the title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme.

## Experimental

An equimolar mixture of 4-benzoyl-5-phenyl-2,3-furandione (1 g) and ethylurea (0.32 g) was heated in boiling benzene for 6 h. After cooling to room temperature the residue was treated with dry ether and the crude product crystallized from *n*-butanol, m.p. 452 K, yield 82%. C<sub>19</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub> requires C 74.98, H 5.30, N 9.21%. Found C 75.03, H 5.35, N 9.14%. IR (cm<sup>-1</sup>): 3100–2870 (aromatic and aliphatic C—H), 1670–1645 (C=O), 1600 (aromatic ring).

### Crystal data

C<sub>19</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>  
*M<sub>r</sub>* = 304.34  
 Monoclinic  
*P*2<sub>1</sub>/*c*  
*a* = 8.4254 (4) Å  
*b* = 17.2278 (6) Å  
*c* = 10.9291 (3) Å  
 $\beta$  = 96.164 (2)°  
*V* = 1577.2 (1) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.282 Mg m<sup>-3</sup>  
*D<sub>m</sub>* not measured

Mo *K*α radiation  
 $\lambda$  = 0.71073 Å  
 Cell parameters from 1489 reflections  
 $\theta$  = 1.5–33°  
 $\mu$  = 0.084 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Needle  
 0.56 × 0.14 × 0.06 mm  
 Colourless

### Data collection

Siemens SMART CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: none  
 8150 measured reflections  
 2756 independent reflections

1241 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.109$   
 $\theta_{\text{max}} = 27.50^\circ$   
 $h = -12 \rightarrow 8$   
 $k = -25 \rightarrow 26$   
 $l = -16 \rightarrow 15$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.068$   
 $wR(F^2) = 0.121$

$(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.18 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.17 \text{ e } \text{Å}^{-3}$

*S* = 1.009  
 2754 reflections  
 273 parameters  
 All H-atom parameters refined  
 $w = 1/[\sigma^2(F_o^2) + (0.0246P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

Extinction correction: *SHELXL*  
 Extinction coefficient: 0.0157 (17)  
 Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. Selected geometric parameters (Å, °)

O1—C2	1.220 (4)	N1—C18	1.482 (5)
O2—C5	1.223 (4)	N2—C3	1.310 (4)
N1—C1	1.344 (4)	N2—C2	1.378 (4)
N1—C2	1.406 (4)		
O1—C2—N1	123.3 (4)	C6—C5—C4	120.2 (3)
O1—C2—N2	119.6 (4)	N1—C18—C19	112.5 (4)
N2—C3—C12	114.9 (3)		

The data collection covered over a hemisphere of reciprocal space by a combination of three sets of exposures; each set had a different  $\varphi$  angle (0, 88 and 180°) for the crystal and each exposure of 10 s covered 0.3° in  $\omega$ . The crystal-to-detector distance was 4 cm and the detector-swing angle was  $-35^\circ$ . Coverage of the unique set is over 99% complete. Crystal decay was monitored by repeating thirty initial frames at the end of data collection and analysing the duplicate reflections, and was found to be negligible.

The structure was solved by direct methods and refined by full-matrix least-squares techniques. All H atoms were located from a difference Fourier map and refined isotropically. C—H distances range from 0.88 (4) to 1.04 (3) Å and  $U_{\text{iso}}$  values for H atoms range from 0.025 (9) to 0.23 (4) Å<sup>2</sup>.

Data collection: *SMART* (Siemens, 1996*a*). Cell refinement: *SAINT* (Siemens, 1996*b*). Data reduction: *SAINT*. Program(s) used to solve structure: *SHELXTL* (Sheldrick, 1996). Program(s) used to refine structure: *SHELXTL*. Molecular graphics: *SHELXTL*. Software used to prepare material for publication: *SHELXTL* and *PARST* (Nardelli, 1995).

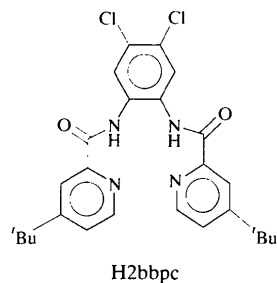
The authors would like to thank the Malaysian Government and Universiti Sains Malaysia for research grant R & D No. 190-9609-2801. SÖ thanks the Universiti Sains Malaysia for a Visiting Post-Doctoral Fellowship.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1134). Services for accessing these data are described at the back of the journal.

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### *N,N'*-(4,5-Dichloro-*o*-phenylene)bis(4-*tert*-butylpyridine-2-carboxamide)

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#### Abstract

In the title compound, C<sub>26</sub>H<sub>28</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>2</sub>, one of the pyrimidine rings is nearly coplanar with the benzene ring whereas the other forms a dihedral angle of 50.9 (1)°.

#### Comment

The design of new metal catalysts to mimic the oxidative activities of metalloporphyrins has continued to be an active area of research. Previous work revealed that diamide tetradentate compounds, such as 1,2-bis-(pyridine-2-carboxamido)benzene (H2bpb) and 4,5-dichloro-1,2-bis(pyridine-2-carboxamido)benzene (H2bpc), form stable complexes with transition metal ions such as Mn<sup>III</sup> and Cr<sup>III</sup>, and found them to be active catalysts for the oxidation of alkenes and alkanes (Chapman *et al.*, 1981). However, attempts to prepare the related ruthenium complexes have failed. This may be due to the low solubility of the amides and their metal complexes in organic solvents. To circumvent the problem, a soluble derivative of H2bpc [H2bbpc] was prepared by introducing a *tert*-butyl group on the pyridine ring (Ko *et al.*, 1995).

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The mean C—N length in the pyridine rings of H2bbpc is 1.336 (4) Å. The N2—C11 and N3—C16 bond distances are longer than the N2—C10 and N3—C17 distances. The C—C lengths observed in the structure show normal values (Allen *et al.*, 1987). One of the pyridine rings (N1) is nearly coplanar with the benzene ring [dihedral angle 2.42 (9)°] and this coplanarity is stabilized by a C—H···O intramolecular hydrogen bond between C12 and O1. The other pyridine ring forms a dihedral angle of 50.9 (1)° with the benzene ring. The crystal structure is stabilized by van der Waals interactions.

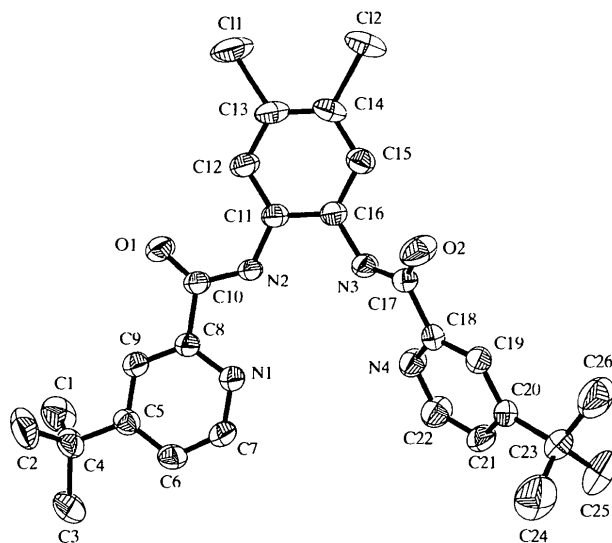


Fig. 1. The structure of the H2bbpc showing 50% probability displacement ellipsoids and the atom-numbering scheme.

#### Experimental

The title compound was synthesized according to the method of Ko *et al.* (1995) and crystallized by slow evaporation of the compound from acetonitrile at room temperature. Only rather small weakly diffracting crystals could be obtained.

#### Crystal data

C<sub>26</sub>H<sub>28</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>2</sub>  
*M<sub>r</sub>* = 499.42

Mo *K*α radiation  
 λ = 0.71073 Å