

Anwar Usman,<sup>a</sup> Ibrahim Abdul Razak,<sup>a</sup> Hoong-Kun Fun,<sup>a\*</sup> Suchada Chantrapromma,<sup>a†</sup> Yun Li,<sup>b</sup> Yan Zhang<sup>b</sup> and Jian-Hua Xu<sup>b</sup>

<sup>a</sup>X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and <sup>b</sup>Department of Chemistry, Nanjing University, Nanjing 210093, People's Republic of China

† Permanent address: Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkla 90112, Thailand.

Correspondence e-mail: hkfun@usm.my

#### Key indicators

Single-crystal X-ray study  
T = 213 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$   
R factor = 0.066  
wR factor = 0.155  
Data-to-parameter ratio = 17.3

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

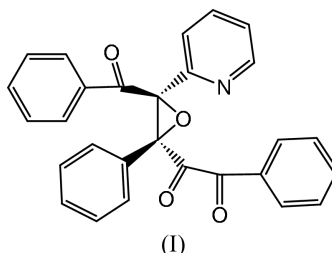
## 2-Benzoyl-3-(1,2-dioxo-2-phenylethyl)-3-phenyl-2-(pyridin-2-yl)oxirane

In the title compound,  $\text{C}_{28}\text{H}_{19}\text{NO}_4$ , the configurations of the substituents attached to the oxirane ring are conditioned by the  $sp^3$  states of the oxirane C atoms. In the packing, the molecules form zigzag molecular chains along the  $b$  direction.

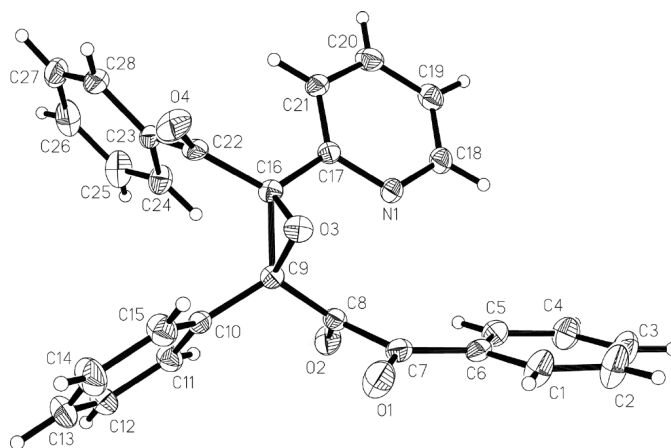
Received 1 August 2002  
Accepted 27 August 2002  
Online 13 September 2002

#### Comment

Photoinduced oxygenation reactions of indolizine derivatives have been investigated intensively in our previous study (Tian *et al.*, 2001). In continuation of that work, we have isolated the title compound, (I), which was obtained from the photo-oxygenation reactions of 1,3-dibenzoyl-2-phenylindolizine. We report here an X-ray crystallographic analysis at 213 K of (I), which was undertaken to establish its conformation and stereochemistry.



The bond lengths and angles observed in (I) (Fig. 1) are within normal ranges (Allen *et al.*, 1987). The values within the oxirane (O3/C9/C16) agree with those of a related structure studied previously (Krishnakumar *et al.*, 2002), except for a slight elongation of the C9–C16 bond [1.509 (3) Å versus 1.488 (4) Å (Krishnakumar *et al.*, 2002)] due to the bulky substituents attached at atoms C9 and C16. The configurations



**Figure 1**

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

of the substituents are conditioned by these two *sp*<sup>3</sup> atoms. Except for the bond angles within the oxirane, the average bond angles subtended at atoms C9 and C16 are 117.2 and 116.8°, respectively, while the two atoms are eclipsed, as determined by the torsion angles C8–C9–C16–C17 = 1.4 (3)° and C10–C9–C16–C22 = 4.7 (3)°.

In the dioxophenylethylene moiety (O1/O2/C1–C9), the two carbonyl groups form O1/C6/C7/C8 and O2/C7/C8/C9 planes. These two planes are twisted out of the phenyl ring by 11.7 (1) and 38.8 (1)°, respectively. The O2/C7/C8/C9 plane and the C10–C15 phenyl ring attached at atom C9 form dihedral angles of 56.1 (1) and 63.6 (2)°, respectively, with the oxirane ring plane.

The pyridine ring (N1/C17–C21) attached at atom C16 is perpendicular to the oxirane ring plane, with a dihedral angle of 88.6 (2)°. The carbonyl group of the benzoyl moiety (O4/C22–C28) attached at the same atom is twisted from its aromatic ring by an angle of 20.8 (1)° and the O4/C16/C22/C23 plane makes a dihedral angle of 61.8 (2)° with the oxirane ring plane.

In the packing, the molecules are interconnected by C21–H21···O4<sup>i</sup> interactions [H21···O4<sup>i</sup> 2.56 Å and C21–H21···O4<sup>i</sup> 129°; symmetry code: (i) 1 – *x*, *y* – ½, ½ – *z*] into zigzag molecular chains along the *b* direction (Fig. 2). These interactions, along with the dipole–dipole and van der Waals interactions, stabilize the packing.

## Experimental

The title compound was prepared by photoinduced oxygenation of 1,3-dibenzoyl-2-phenylindolizine in acetonitrile and was isolated by column chromatography. Single crystals for X-ray measurement were obtained by slow evaporation of the solvent from a petroleum ether–ethyl acetate (5:1 *v/v*) solution.

### Crystal data

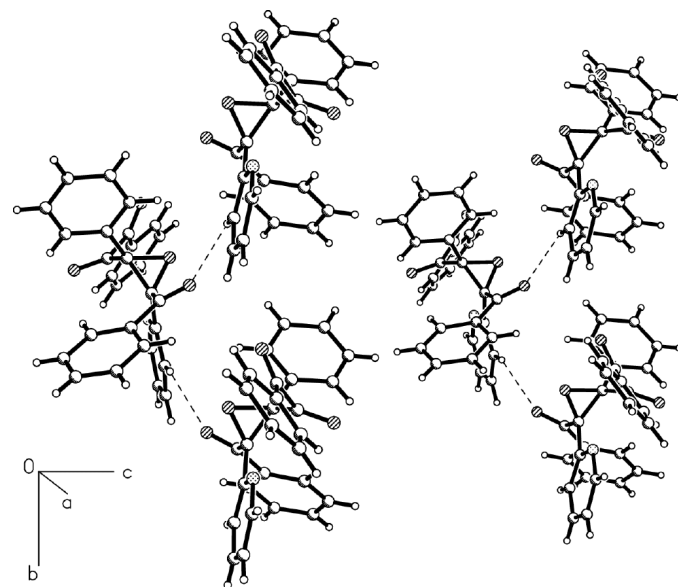
C <sub>28</sub> H <sub>19</sub> NO <sub>4</sub>	<i>D<sub>x</sub></i> = 1.330 Mg m <sup>−3</sup>
<i>M<sub>r</sub></i> = 433.44	Mo <i>K</i> α radiation
Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>c</i>	Cell parameters from 7367 reflections
<i>a</i> = 13.1513 (4) Å	<i>θ</i> = 2.6–28.3°
<i>b</i> = 9.7358 (3) Å	<i>μ</i> = 0.09 mm <sup>−1</sup>
<i>c</i> = 16.9960 (5) Å	<i>T</i> = 213 (2) K
<i>β</i> = 95.859 (1)°	Slab, colorless
<i>V</i> = 2164.8 (1) Å <sup>3</sup>	0.38 × 0.34 × 0.16 mm
<i>Z</i> = 4	

### Data collection

Siemens SMART CCD area-detector diffractometer	<i>R</i> <sub>int</sub> = 0.110
<i>ω</i> scans	<i>θ</i> <sub>max</sub> = 28.3°
12 406 measured reflections	<i>h</i> = −10 → 17
5164 independent reflections	<i>k</i> = −12 → 12
2808 reflections with <i>I</i> > 2σ( <i>I</i> )	<i>l</i> = −22 → 22

### Refinement

Refinement on <i>F</i> <sup>2</sup>	<i>w</i> = 1/[σ <sup>2</sup> ( <i>F</i> <sub>o</sub> <sup>2</sup> )]
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.066	where <i>P</i> = ( <i>F</i> <sub>o</sub> <sup>2</sup> + 2 <i>F</i> <sub>c</sub> <sup>2</sup> )/3
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.156	(Δ/σ) <sub>max</sub> = 0.001
<i>S</i> = 0.79	Δρ <sub>max</sub> = 0.34 e Å <sup>−3</sup>
5164 reflections	Δρ <sub>min</sub> = −0.28 e Å <sup>−3</sup>
299 parameters	Extinction correction: <i>SHELXTL</i>
H-atom parameters constrained	Extinction coefficient: 0.021 (2)



**Figure 2**

Part of the packing of the title compound, viewed down the *a* axis, showing the zigzag molecular chains along the *b* direction.

**Table 1**

Selected geometric parameters (Å, °).

O3–C9	1.434 (2)	O3–C16	1.441 (2)
O3–C9–C10	117.42 (16)	O3–C16–C17	115.18 (15)
C10–C9–C16	120.90 (17)	C17–C16–C9	120.12 (17)
O3–C9–C8	113.57 (15)	O3–C16–C22	112.92 (16)
C10–C9–C8	114.73 (17)	C17–C16–C22	117.30 (17)
C16–C9–C8	119.33 (16)	C9–C16–C22	118.55 (16)

The H atoms were fixed geometrically and were treated as riding on their parent C atoms, with C–H = 0.93 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT* and *SADABS* (Sheldrick, 1996); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

The authors thank the Malaysian Government and Universiti Sains Malaysia for research grant R&D No. 305/PFIZIK/610961. AU thanks Universiti Sains Malaysia for a Visiting Postdoctoral Fellowship.

## References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Krishnakumar, R. V., Subha Nandhini, M., Renuga, S., Natarajan, S., Selvaraj, S. & Perumal, S. (2002). *Acta Cryst.* **E58**, o504–o505.
- Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Spek, A. L. (1990). *Acta Cryst.* **A46**, C-34.