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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
 Mean $\sigma(\text{C}-\text{C}) = 0.011\text{ \AA}$
 R factor = 0.084
 wR factor = 0.221
 Data-to-parameter ratio = 14.3

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

2,2'-Sulfonylbis(2-benzoyl-3-phenyloxirane)

The X-ray crystallographic study of the title compound, $\text{C}_{30}\text{H}_{22}\text{O}_6\text{S}$, demonstrates the relative configuration between the aryl and aroyl groups (*cis*) on one hand, and that between the two oxirane rings (*cis*) on the other. The crystal packing is characterized by a $\text{C}-\text{H}\cdots\text{O}$ interaction and $\text{C}\cdots\text{O}$ short contacts.

Comment

Organic synthesis of small ring heterocycles, such as oxiranes, assumes great importance in view of their reactivity towards a host of reagents and the synthetic potential associated with them. Details of chemical synthesis, NMR studies and preliminary crystallographic data for the title compound, (I), have already been reported (Renuga *et al.*, 1999). Interestingly, (I) exhibits stereoisomerism and the difficulty in ascertaining the configuration arises because one of the C atoms of each oxirane ring is a chiral center, as a result of which the molecule further exhibits diastereoisomerism with respect to the oxirane rings. Recently, the crystal structure of 2,2'-thio-bis[2-benzoyl-3-(4-chlorophenyl)oxirane] (Krishnakumar *et al.*, 2002) was elucidated in our laboratory.

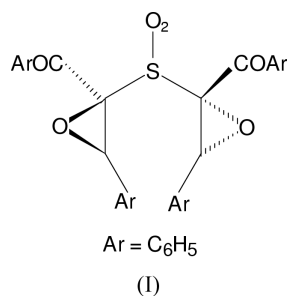


Fig. 1 shows the atom-numbering scheme adopted for (I). This study demonstrates the relative configuration between the aryl and aroyl groups (*cis*) on one hand and that between the two oxirane rings (*cis*) on the other. The configuration of (I), which is symmetrical in solution in the absence of intermolecular interactions, assumes an unsymmetrical form in the solid state. The absence of symmetry is probably necessitated by the optimum packing considerations, which bring different oxirane rings in proximity, unlike in solution.

Fig. 2 shows the arrangement of molecules in layers parallel to the (020) plane, viewed down the *a* axis. The packing features of (I) are distinctly different from those of 2,2'-thio-bis[2-benzoyl-3-(4-chlorophenyl)oxirane], as its packing is determined, not only by the $\text{C}-\text{H}\cdots\text{O}$, but also by the $\text{Cl}\cdots\text{Cl}$ interactions. The molecules of (I) do not interact directly among themselves, except for the presence of a $\text{C}-\text{H}\cdots\text{O}$

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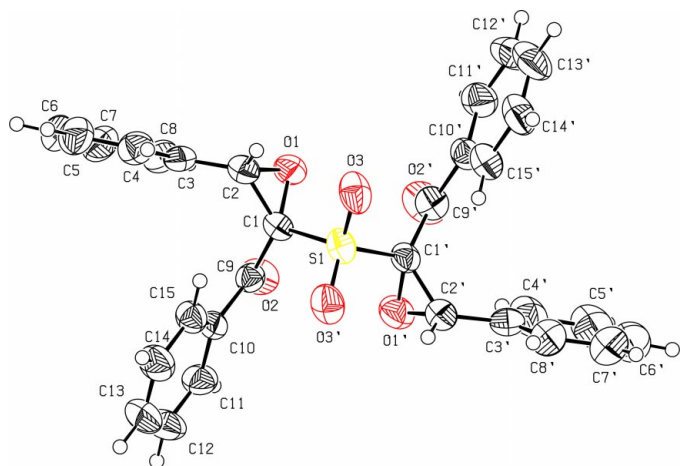


Figure 1
View of (I), showing the atom-numbering scheme adopted, with displacement ellipsoids drawn at the 50% probability level.

hydrogen bond. In addition, the structure is stabilized by a number of C...O short contacts (see Table 1). Since the molecules of (I) have aromatic rings, C—H... π interactions are expected to play a dominant role in stabilizing the crystal packing. An investigation (Malone *et al.*, 1997) on the nature of C—H... π interactions, using the Cambridge Structural Database (Allen & Kennard, 1993) and theoretical calculations, suggest six possible forms of interactions between an H atom and an aromatic ring. A recent database study (Umezawa *et al.*, 1998) on the nature of C—H... π interactions shows that these interactions also contribute significantly to the optimum packing modes observed in the crystal structures of organic compounds. The observed H... π distances in (I) are 3.002 and 3.003 Å (below a cut off value of 3.05 Å), with C—H... π angles 158 and 133°.

Experimental

Colourless single crystals of (I) were obtained as transparent needles from a saturated solution in methanol, by slow evaporation at room temperature.

Crystal data

$C_{30}H_{22}O_6S$	$D_x = 1.337 \text{ Mg m}^{-3}$
$M_r = 510.54$	Cu $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25 reflections
$a = 13.228 (3) \text{ \AA}$	$\theta = 14\text{--}27^\circ$
$b = 11.754 (6) \text{ \AA}$	$\mu = 1.50 \text{ mm}^{-1}$
$c = 18.659 (5) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 119.05 (2)^\circ$	Needle, colourless
$V = 2536.2 (16) \text{ \AA}^3$	$0.40 \times 0.34 \times 0.24 \text{ mm}$
$Z = 4$	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{\text{int}} = 0.019$
ω - 2θ scans	$\theta_{\text{max}} = 69.9^\circ$
Absorption correction: ψ scan (North <i>et al.</i> , 1968)	$h = 0 \rightarrow 16$
$T_{\text{min}} = 0.576$, $T_{\text{max}} = 0.698$	$k = -14 \rightarrow 0$
5012 measured reflections	$l = -22 \rightarrow 19$
4795 independent reflections	2 standard reflections every 100 reflections
3365 reflections with $I > 2\sigma(I)$	intensity decay: <1%

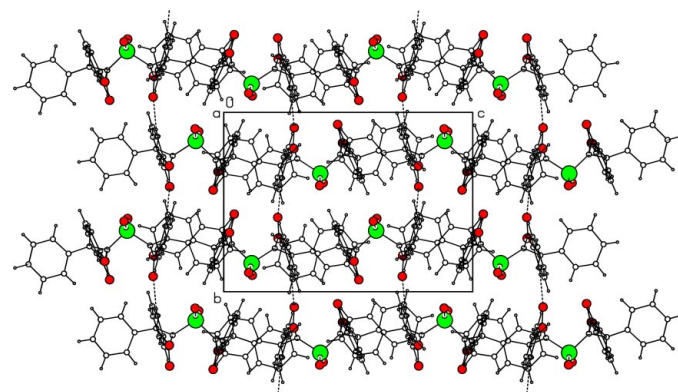


Figure 2
Packing diagram, showing the arrangement of molecules in layers parallel to the (020) plane, viewed down the a axis.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + 14.8815P]$
$R[F^2 > 2\sigma(F^2)] = 0.084$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.221$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.12$	$\Delta\rho_{\text{max}} = 0.43 \text{ e \AA}^{-3}$
4795 reflections	$\Delta\rho_{\text{min}} = -0.45 \text{ e \AA}^{-3}$
335 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.00103 (5)

Table 1

Contact distances (Å).

C4...O3 ⁱ	3.25 (1)	C14...O1 ⁱⁱⁱ	3.47 (1)
C5...O3 ^{ri}	3.24 (1)	C7'...O1 ^v	3.29 (1)
C7...O1 ⁱⁱⁱ	3.27 (1)	C8'...O1 ^v	3.37 (1)
C8...O2 ⁱⁱⁱ	3.46 (1)	C14'...C12 ^{vi}	3.41 (1)
C12...C14 ^{iv}	3.41 (1)		

Symmetry codes: (i) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$; (ii) $x, \frac{3}{2} - y, \frac{1}{2} + z$; (iii) $1 - x, y - \frac{1}{2}, \frac{3}{2} - z$; (iv) $1 + x, \frac{3}{2} - y, \frac{1}{2} + z$; (v) $x, \frac{3}{2} - y, z - \frac{1}{2}$; (vi) $x - 1, \frac{3}{2} - y, z - \frac{1}{2}$.

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C15—H15...O2 ⁱ	0.93	2.60	3.458 (8)	154

Symmetry code: (i) $1 - x, y - \frac{1}{2}, \frac{3}{2} - z$.

All H atoms were included in calculated positions with distances of 0.93 (for sp^2 C—H) and 0.98 Å (for sp^3 C—H). In the refinement, they were included as riding, with U_{iso} values equal to $1.2U_{\text{eq}}$ of the carrier atom.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL97*.

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