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## Key indicators

Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.042  
 $wR$  factor = 0.115  
Data-to-parameter ratio = 10.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

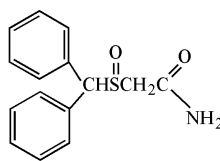
## 2-(Benzhydrylsulfinyl)acetamide

The title compound,  $\text{C}_{15}\text{H}_{14}\text{NO}_2\text{S}$ , was prepared by the esterification of benzhydrylthioacetic acid, followed by amidation and oxidation. There are two independent molecules in the asymmetric unit.

Received 5 January 2004  
Accepted 19 January 2004  
Online 14 February 2004

## Comment

Novel acetamides have been discovered to have useful pharmaceutical activity on the central nervous system (Louis, 1978). They may be prepared by reacting the corresponding ester or acid halide with the appropriately substituted amine. The structure of the title compound, (I), is reported here as an early result in our study of this new series of compounds.



(I)

In the crystal structure of (I), there are two independent molecules in the asymmetric unit (Fig. 1 and Table 1). The crystal structure is shown in Fig. 2. There is an intermolecular hydrogen bond between O1 and N1 with an  $\text{O1}\cdots\text{N1}$  distance of 2.96 Å.

## Experimental

Thionyl chloride (2 ml) was added into a benzene solution of benzhydrylthioacetic acid (1.955 g, 7 mmol) at room temperature,

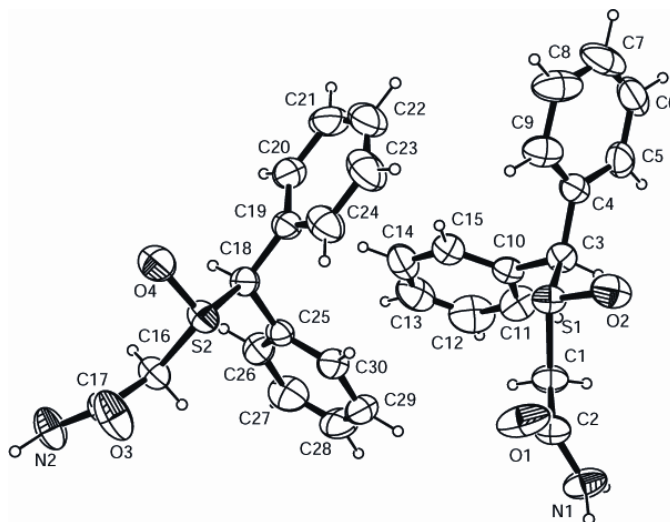
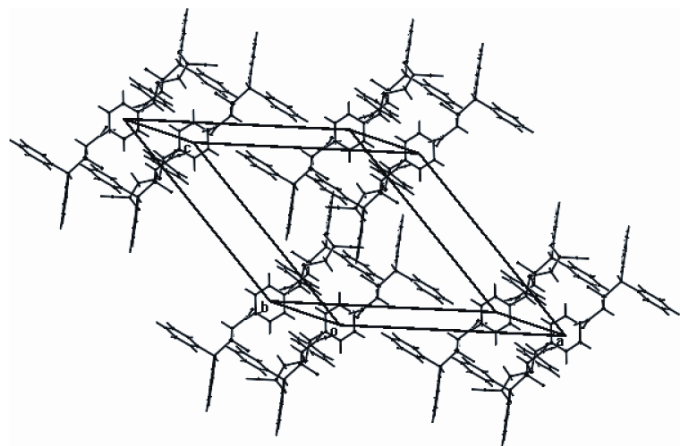


Figure 1

The molecular structure of the asymmetric unit of (I), with 50% probability displacement ellipsoids and the atom numbering scheme.



**Figure 2**  
The crystal structure of (I).

and the mixture was heated for 1 h. The resulting chloride was filtered off and dissolved in methanol (10 ml) and, after refluxing for 1 h, ammonia was bubbled in at a high flow rate for 1 h. The solvent was evaporated and the residue was dissolved in ethanol. After 3 d, crystals of (I) were obtained from an ethanol solution.

#### Crystal data

$C_{15}H_{15}NO_2S$   
 $M_r = 273.35$   
Monoclinic,  $P2_1/n$   
 $a = 20.961(1) \text{ \AA}$   
 $b = 9.7061(5) \text{ \AA}$   
 $c = 20.894(1) \text{ \AA}$   
 $\beta = 139.336(1)^\circ$   
 $V = 2770.0(3) \text{ \AA}^3$   
 $Z = 8$

$D_x = 1.311 \text{ Mg m}^{-3}$   
Mo  $K\alpha$  radiation  
Cell parameters from 16675  
reflections  
 $\theta = 2.3\text{--}27.4^\circ$   
 $\mu = 0.23 \text{ mm}^{-1}$   
 $T = 298(1) \text{ K}$   
Prism, colorless  
 $0.29 \times 0.28 \times 0.20 \text{ mm}$

#### Data collection

Rigaku R-AXIS RAPID  
diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)  
 $T_{\min} = 0.842$ ,  $T_{\max} = 0.955$   
47104 measured reflections

6218 independent reflections  
3764 reflections with  $F^2 > 2\sigma(F^2)$   
 $R_{\text{int}} = 0.027$   
 $\theta_{\max} = 27.4^\circ$   
 $h = -27 \rightarrow 27$   
 $k = -12 \rightarrow 12$   
 $l = -27 \rightarrow 27$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.115$   
 $S = 1.00$   
3776 reflections  
373 parameters

H-atom parameters constrained  
 $w = (4F_o^2)/[0.002F_o^2 + 1.6\sigma(F_o^2)]$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.41 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.30 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

S1—O2	1.485 (3)	N1—C2	1.317 (5)
S1—C1	1.797 (2)	N2—C17	1.322 (5)
S1—C3	1.838 (2)	C1—C2	1.517 (3)
S2—O4	1.487 (3)	C3—C4	1.512 (3)
S2—C16	1.789 (2)	C3—C10	1.515 (5)
S2—C18	1.837 (2)	C16—C17	1.515 (3)
O1—C2	1.226 (4)	C18—C19	1.520 (3)
O3—C17	1.222 (3)	C18—C25	1.513 (4)
O2—S1—C1—C2	60.8 (3)	O4—S2—C16—C17	−65.0 (3)
C3—S1—C1—C2	169.8 (3)	C18—S2—C16—C17	−172.8 (3)
O2—S1—C3—C4	−60.3 (3)	O4—S2—C18—C19	65.3 (3)
O2—S1—C3—C10	172.7 (2)	O4—S2—C18—C25	−168.4 (2)
C1—S1—C3—C4	−170.3 (3)	C16—S2—C18—C19	174.4 (3)
C1—S1—C3—C10	62.8 (2)	C16—S2—C18—C25	−59.3 (2)

All the H atoms were placed in calculated positions and then allowed for as riding, with C—H and N—H distances of 0.95  $\text{\AA}$ .

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2003); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 1996); *ORTEP-3* (Version 1.06; Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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