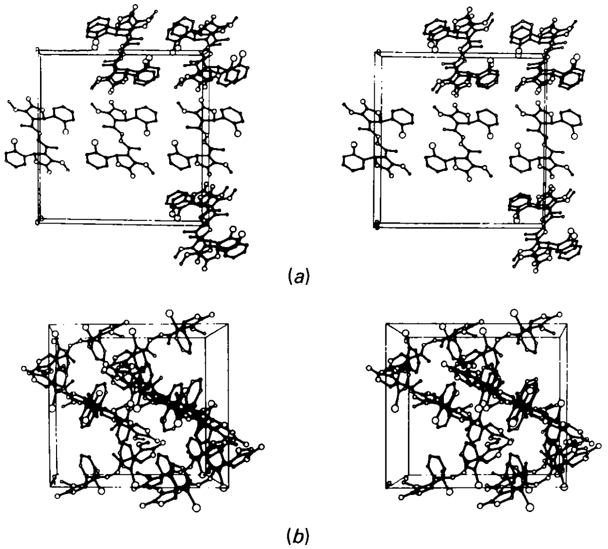

Fig. 2. Stereoscopic views of the crystal packing of (*a*) isomer (I) and (*b*) isomer (II).

range 435—483 K (Kurihara, Nasu, Inoue & Ishida, 1982). This observation is comparable with the result of the energy calculation that the twisted conformation around the =N—N= bond is more stable than the planar one.

There are no intermolecular contacts closer than the sum of the appropriate van der Waals radii for both isomers in their crystal structures.

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Structure of 2-(Methylsulphinyl)-1,2-diphenylethyl Acetate, $C_{17}H_{18}O_3S$

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Abstract. $M_r = 302{\cdot}4$, monoclinic, space group $P2_1/c$, $a = 8{\cdot}878\ (1)$, $b = 21{\cdot}703\ (4)$, $c = 8{\cdot}408\ (1)$ Å, $\beta = 93{\cdot}47\ (1)°$, $V = 1617{\cdot}1\ (4)$ Å^3, $Z = 4$, $D_x = 1{\cdot}242$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}197$ mm^{-1}, $F(000) = 640$. Final $R = 0{\cdot}082$ for 2496 observed reflections. The three chiral centres, C(1),C(2),S, are *S,R,S* (or *R,S,R*) respectively.

Introduction. The present study is a continuation of the investigations we are carrying out into the structure of sulphoxides.

Experimental. Crystals prepared by Dr Rodriguez-Ramos; colourless crystal, 0·2 × 0·3 × 0·2 mm, mounted at random on a Philips PW1100 four-circle diffractometer, was used for both cell-parameter determinations and intensity measurements; cell dimensions obtained by a least-squares fit of settings for 54 reflections ($\pm hkl$), intensities recorded in $\omega/2\theta$ scan mode with θ ranging between 2 and 35°, graphite-monochromated Mo $K\alpha$ radiation, 4729 unique reflections, 2496 considered observed with $I > 2\sigma(I)$ and retained for use in structure analysis; intensities and ω angles of two reference reflections measured periodically every 90 min showed no appreciable variation during course of data collection; Lorentz and polarization but no absorption correction; direct-methods program *MULTAN* 78 (Main, Woolfson,

0108-2701/83/040473-03$01.50

Hull, Lessinger, Germain & Declercq, 1978) used to calculate phases for $|E|$ values greater than 1·5; phase set with highest combined figure of merit selected and the E map calculated with these phases revealed the positions of the 21 non-H atoms; the positions of the H atoms were found where expected in a difference Fourier synthesis after refinement of positional and anisotropic thermal parameters of non-H atoms; least-squares refinement of a scale factor, atomic coordinates, anisotropic temperature parameters for non-H atoms and isotropic for H atoms gave $R = 0{\cdot}082$, $R_w = 0{\cdot}079$ for 2233 observed reflections; refinement conducted until all atomic-parameter shifts were smaller than their standard deviations; weights calculated (Martinez-Ripoll & Cano, 1975) as $w = K/\sigma^2$, $\sigma = a + b|F_o|$ and $K = 0{\cdot}547$, $a = 2{\cdot}983$, $b = -3{\cdot}521$ when $|F_o| = 0{\cdot}25$–$0{\cdot}61$, $a = 0{\cdot}726$, $b = 0{\cdot}166$ when $|F_o| = 0{\cdot}61$–$4{\cdot}0$, $a = 2{\cdot}053$, $b = -0{\cdot}177$ when $|F_o| = 4{\cdot}0$–$8{\cdot}70$, $a = 0{\cdot}449$, $b = 0{\cdot}013$ when $|F_o| > 8{\cdot}70$; no trends in $\sin\theta/\lambda$ observed, atomic scattering factors taken from *International Tables for X-ray Crystallography* (1974), computations carried out with programs of the XRAY 70 system (Stewart, Kundell & Baldwin, 1970) on a 1108 Univac computer.

Discussion. Final atomic positional parameters are given in Table 1.* Interatomic distances, bond angles and torsion angles are presented in Table 2.

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (×10⁴) *for non*-H *atoms, with e.s.d.'s in parentheses*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.\cos(a_i,a_j).$$

	x	y	z	U_{eq}(Å²)
S	0·87951 (13)	0·66587 (5)	0·64950 (14)	562 (4)
O(1)	0·58508 (29)	0·60627 (12)	0·64490 (30)	476 (9)
O(2)	0·82249 (43)	0·71683 (18)	0·74701 (44)	889 (16)
O(3)	0·38599 (37)	0·64989 (15)	0·75359 (38)	696 (12)
C(1)	0·58657 (43)	0·65576 (16)	0·53141 (46)	422 (12)
C(2)	0·74776 (42)	0·65905 (18)	0·47313 (46)	430 (12)
C(3)	1·03617 (66)	0·69583 (33)	0·54908 (93)	796 (24)
C(4)	0·79261 (41)	0·60705 (19)	0·36924 (47)	450 (13)
C(5)	0·81025 (51)	0·54740 (21)	0·42655 (63)	574 (16)
C(6)	0·85131 (59)	0·50030 (26)	0·32607 (81)	754 (22)
C(7)	0·87506 (59)	0·51238 (29)	0·16976 (78)	831 (23)
C(8)	0·85934 (58)	0·57102 (32)	0·11268 (66)	816 (23)
C(9)	0·81890 (51)	0·61827 (26)	0·21085 (55)	605 (17)
C(10)	0·46925 (40)	0·64808 (17)	0·39662 (45)	412 (11)
C(11)	0·44211 (53)	0·69672 (23)	0·29176 (61)	608 (17)
C(12)	0·33643 (56)	0·69140 (27)	0·16511 (63)	699 (19)
C(13)	0·25154 (59)	0·63948 (30)	0·14636 (66)	733 (21)
C(14)	0·27579 (59)	0·59087 (26)	0·24997 (63)	705 (19)
C(15)	0·38459 (50)	0·59539 (21)	0·37403 (53)	544 (15)
C(16)	0·47957 (45)	0·61017 (20)	0·75536 (47)	496 (13)
C(17)	0·49833 (82)	0·55870 (36)	0·87138 (81)	737 (23)

Table 2. *Molecular geometry*

(*a*) Intramolecular distances (Å)			
C(4)–C(5)	1·387 (6)	C(10)–C(1)	1·501 (5)
C(5)–C(6)	1·389 (8)	C(1)–C(2)	1·542 (5)
C(6)–C(7)	1·369 (9)	C(2)–C(4)	1·495 (6)
C(7)–C(8)	1·364 (9)	C(1)–O(1)	1·437 (4)
C(8)–C(9)	1·379 (8)	O(1)–C(16)	1·361 (5)
C(9)–C(4)	1·387 (6)	C(16)–C(17)	1·486 (9)
C(10)–C(11)	1·387 (6)	C(16)–O(3)	1·196 (5)
C(11)–C(12)	1·381 (7)	C(2)–S	1·838 (4)
C(12)–C(13)	1·359 (8)	S–O(2)	1·484 (4)
C(13)–C(14)	1·377 (8)	S–C(3)	1·792 (7)
C(14)–C(15)	1·381 (7)		
C(15)–C(10)	1·376 (6)		

(*b*) Intramolecular angles (°)			
C(4)–C(5)–C(6)	120·3 (5)	C(10)–C(1)–C(2)	112·3 (3)
C(5)–C(6)–C(7)	120·3 (5)	C(10)–C(1)–O(1)	112·6 (3)
C(6)–C(7)–C(8)	119·9 (6)	C(1)–O(1)–C(16)	116·1 (3)
C(7)–C(8)–C(9)	120·5 (6)	O(1)–C(16)–O(3)	122·9 (4)
C(8)–C(9)–C(4)	120·6 (5)	O(1)–C(16)–C(17)	110·3 (4)
C(9)–C(4)–C(5)	118·4 (4)	O(3)–C(16)–C(17)	126·8 (4)
C(10)–C(11)–C(12)	120·7 (5)	O(1)–C(1)–C(2)	107·0 (3)
C(11)–C(12)–C(13)	120·3 (5)	C(1)–C(2)–C(4)	115·8 (3)
C(12)–C(13)–C(14)	119·9 (5)	C(1)–C(2)–S	107·7 (3)
C(13)–C(14)–C(15)	119·9 (5)	C(4)–C(2)–S	110·7 (3)
C(14)–C(15)–C(10)	121·0 (4)	C(2)–S–O(2)	106·5 (2)
C(15)–C(10)–C(11)	118·1 (4)	C(2)–S–C(3)	97·1 (3)
C(5)–C(4)–C(2)	122·0 (4)	O(2)–S–C(3)	106·9 (3)
C(9)–C(4)–C(2)	119·6 (4)		
C(11)–C(10)–C(1)	118·8 (4)		
C(15)–C(10)–C(1)	123·1 (4)		

(*c*) Torsion angles (°)			
C(12)–C(11)–C(10)–C(1)	−179·3 (4)	C(1)–C(2)–C(4)–C(5)	−67·1 (5)
C(11)–C(10)–C(1)–O(1)	170·2 (4)	C(2)–C(4)–C(5)–C(6)	179·7 (4)
C(10)–C(1)–O(1)–C(16)	−81·5 (4)	C(2)–C(1)–O(1)–C(16)	154·7 (3)
C(1)–O(1)–C(16)–O(3)	4·9 (6)	C(10)–C(1)–C(2)–S	−178·2 (3)
C(1)–O(1)–C(16)–C(17)	−175·9 (4)	C(1)–C(2)–S–C(3)	−160·4 (3)
C(11)–C(10)–C(1)–C(2)	−68·9 (4)	C(1)–C(2)–S–O(2)	−50·4 (3)
C(10)–C(1)–C(2)–C(4)	−53·7 (4)		

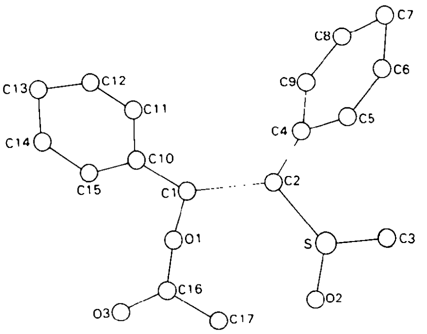

Fig. 1. Labelling scheme for the title compound.

The molecule consists of a phenyl and an acetoxy group and a phenyl and a methylsulphinyl group attached to C(1) and C(2) respectively. The labelling sequence in the molecule is given in Fig. 1.

The average C–C bond lengths in the C(4)–C(9) and C(10)–C(15) phenyl rings are 1·382 (5) and 1·378 (5) Å respectively, these values being comparable with the values usually found for C–C distances in aromatic rings [1·395 (3) Å].

The values in the other groups are similar to those observed in compounds with similar specific groups (Hoyos-Guerrero, Martínez-Carrera & García-Blanco, 1983; Rivera & Sheldrick, 1981; Vega, López-Castro & Márquez, 1981) and do not merit special comment; the only significant difference is found for the distance

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38256 (35 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

S—O(2), 1·484 (4) Å, which is slightly shorter than that [1·504 (2) Å] found in 2-(methylsulphinyl)-1-phenylethanol (Hoyos-Guerrero *et al.*, 1983), presumably due to the intermolecular hydrogen bond present in the latter compound. Slight differences are observed in angles, which are more influenced by packing and conformation.

The chain has an approximately planar zigzag part comprising C(10), C(1), C(2) and S with a maximum deviation of 0·016 (4) Å from the weighted least-squares plane.

The phenyl ring C(4)—C(9) does not deviate significantly from planarity: $\sum(\Delta/\sigma)^2 = 3\cdot5$, total puckering amplitude $Q = 0\cdot008$ (5) Å. In contrast, the deviations observed for ring C(10)—C(15) are statistically significant: $\sum(\Delta/\sigma)^2 = 22\cdot4$, $Q = 0\cdot024$ (5) Å; however, this distortion, which corresponds to a twisted conformation with a pseudo twofold axis crossing the C(11)—C(12) and C(14)—C(15) sides, is probably not real. Considering the two phenyl rings, the corresponding bond angles in them are not significantly different, indicating that the angle deformations produced by the substituents in the two phenyl rings are equal.

The phenyl groups are markedly twisted with respect to the chain with torsion angles C(11)—C(10)—C(1)—C(2) = −68·9 (4) and C(5)—C(4)—C(2)—C(1) = −67·1 (5)°; the acetoxy and methylsulphinyl groups are also twisted with respect to the chain, but this twisting is much smaller as indicated by the torsion angles C(2)—C(1)—O(1)—C(16) = 154·7 (3) and C(1)—C(2)—S—C(3) = −160·4 (3)°.

The configuration around the chiral centres C(1), C(2) and S can be deduced from the Newman projections of Fig. 2. The conformation about C(1)—C(2) is such that the two phenyl groups are in synclinal orientation; S is antiperiplanar to C(10), synclinal to H(1) and synclinal to O(1). The deviation from the theoretical 60° torsion angle between the two phenyl groups is presumably the result of electrostatic attraction between S and O(1), S···O(1) = 2·915 (3) Å, the approach of the phenyl rings to each other made possible by their relative orientation. In the projection along S—C(2), the methyl group C(3) is antiperiplanar to C(1) and synclinal to the phenyl group C(4)—C(9), in agreement with the values determined in similar compounds (Kodama, Nishihata & Sishio, 1977). Thus the configuration around the chiral centres C(1), C(2) and S is *RSR* for the molecule assumed to be in the general position.

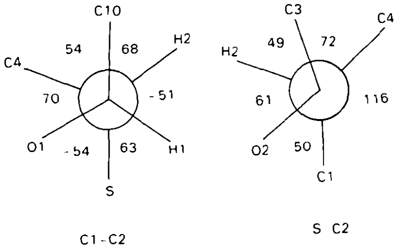

Fig. 2. Some Newman projections (e.s.d.'s 0·3–0·6°).

The molecules are packed in the structure by normal van der Waals interactions.

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