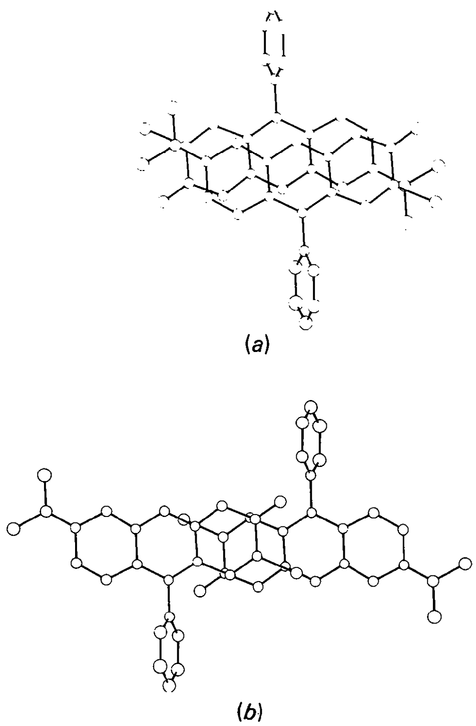

Fig. 3. The relative orientation of centrosymmetrically related dye molecules. (*a*) The molecule with coordinates *x,y,z* shown above that with coordinates $1-x$, $-1-y$, $1-z$. (*b*) The molecule with coordinates $1-x$, $-y$, $1-z$ above that with coordinates *x,y,z*.

characteristic of *J* or staircase aggregates. Thus, the present structure may be described as a combination of both types. The protruding phenyl group has caused separation of the dye layers, but has not entirely prevented the extensive overlap of pairs of dye molecules characteristic of *H* aggregates. Further, because of its size and twist relative to the dye plane, the phenyl ring yields gaps in the structure which are available to be filled by solvent molecules. A structure containing solvent molecules is not a favored candidate for photovoltaic applications since loss of solvent is expected to have the same effect on conductivity as a disordering phase transition. To prevent both solvation and mixed-aggregate formation, slightly smaller out-of-plane substituents at both the 9 and 10 positions are suggested.

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Structures of 1,3-Dicyclohexyl-1-(1*H*-indol-3-ylacetyl)urea, $C_{23}H_{31}N_3O_2$ (I), and 3-Cyclohexyl-1-[2-(1*H*-indol-3-yl)ethyl]urea, $C_{17}H_{23}N_3O$ (II)

By Toshimasa Ishida, Masahiro Yamashita, Hideko Takai and Masatoshi Inoue

Department of Physical Chemistry, Osaka College of Pharmacy, 2-10-65 *Kawai, Matsubara, Osaka* 580, *Japan*

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Abstract. (I): $M_r = 381{\cdot}5$, $P2_1/a$, $a = 9{\cdot}527\,(2)$, $b = 21{\cdot}437\,(5)$, $c = 11{\cdot}046\,(3)$ Å, $\beta = 92{\cdot}05\,(4)°$, $V = 2254\,(1)$ Å^3, $Z = 4$, $D_m = 1{\cdot}123\,(1)$, $D_x = 1{\cdot}124$ Mg m^{-3}, $\lambda(\mathrm{Cu}\,K\alpha) = 1{\cdot}5418$ Å, $\mu(\mathrm{Cu}\,K\alpha) = 5{\cdot}39$ cm^{-1}, $F(000) = 824$, $T = 294$ K, R and $R_w = 0{\cdot}084$ and $0{\cdot}105$ for 3418 non-zero reflections. (II):

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$M_r = 285{\cdot}4$, $P2_1/a$, $a = 9{\cdot}127\,(1)$, $b = 12{\cdot}391\,(1)$, $c = 28{\cdot}017\,(2)$ Å, $\beta = 97{\cdot}78\,(2)°$, $V = 3139{\cdot}2\,(6)$ Å^3, $Z = 8$, $D_m = 1{\cdot}201\,(2)$, $D_x = 1{\cdot}208$ Mg m^{-3}, $\lambda(\mathrm{Cu}\,K\alpha) = 1{\cdot}5418$ Å, $\mu(\mathrm{Cu}\,K\alpha) = 5{\cdot}70$ cm^{-1}, $F(000) = 1232$, $T = 294$ K, R and $R_w = 0{\cdot}106$ and $0{\cdot}119$ for 2493 independent non-zero reflections. Three rings in compound (I) are arranged trigonally to one another, and the molecules form a hexagonally shaped molecular column along the a axis. Two crystallographically independent molecules in compound (II) take almost the same extended conformations, and form hydrophobic double layers perpendicular to the c axis.

Introduction. In order to investigate the effect of an imide or urea group on the spectroscopic properites of the indole ring, the two title compounds (I) and (II) were synthesized by the reaction of 3-indolylacetic acid and tryptamine with *N,N'*-dicyclohexylcarbodiimide, respectively. These compounds showed different spectral properties to each other. In the UV spectra of the absorption region of indole ring (245–310 nm), (I) showed the hypso- and hypochromic effects and (II) showed the batho- and hypochromic effects compared with their component molecules. Further, the fluorescence quenching of (I) and the enhancement of (II) were observed in the 310–450 nm regions of their emission spectra (excitation at 290 nm). These would result from the different conformations of both the molecules and the different association modes of the indole ring with the imide and urea groups.

The aim of this investigation is to determine the molecular conformations and the crystal packing of (I) and (II).

Experimental. Crystallized from ethanol–*n*-hexane-(1:1, *v*/*v*) as transparent platelets (I) or from ethanol as transparent needles (II), $0{\cdot}6 \times 0{\cdot}2 \times 0{\cdot}4$ mm (I), $0{\cdot}1 \times 0{\cdot}4 \times 0{\cdot}05$ mm (II); Rigaku automated four-circle diffractometer, graphite monochromator, cell parameters by least-squares fit to 2θ and -2θ values of 25 independent reflections; D_m by flotation in CCl_4/C_6H_6; intensity data up to $2\theta = 130°$, ω–2θ scans, scan speed 4° (2θ) min^{-1}, scan width (2θ) $(1{\cdot}2 + 0{\cdot}15\tan\theta)°$ at 40 kV and 150 mA; h 0–11, k 0–25, l −12–12 (I), h 0–9, k 0–12, l −28–28 (II); 3418 observed (392 with $I = 0$) (I), 2493 observed (2812 with $I = 0$) (II); four reference reflections monitored at 100-reflection intervals showed no intensity deterioration; Lorentz and polarization corrections applied, absorption ignored; structures for both compounds solved by direct methods with *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), refined by block-diagonal least-squares with anisotropic thermal parameters for all non-H atoms; H atoms located from difference Fourier map, included in the refinement with isotropic thermal parameters; $\sum w(|F_o| - |F_c|)^2$ minimized, $w = 0{\cdot}5942$ for $F_o = 0{\cdot}0$, $w = 1{\cdot}0/[\sigma^2(F_o) + 0{\cdot}1485|F_o| + 0{\cdot}0069|F_o|^2]$ for $F_o > 0{\cdot}0$, where $\sigma(F_o)$ is the standard deviation based on counting statistics (I), $w = 1{\cdot}0$ for $0 < F_o \leq 36{\cdot}0$, $w = 1{\cdot}0/[1{\cdot}0 + 0{\cdot}227\,(F_o - 36{\cdot}0)]$ for $F_o > 36{\cdot}0$ (II); atomic scattering factors from *International Tables for X-ray Crystallography* (1974); $(\Delta/\sigma)_{\max} = \frac{1}{4}$(I), $\frac{1}{3}$(II); final $\Delta\rho$ excursions $\pm 0{\cdot}3$ (I), $\pm 0{\cdot}4$ (II) e Å^{-3}; all numerical calculations made on an ACOS-900 computer at the Computation Center of Osaka University using *The Universal Crystallographic Computing System* (1979).*

Discussion. The final atomic parameters of non-H atoms are listed in Table 1. Perspective views of the molecular conformations, along with the bond lengths and angles between non-H atoms, are shown in Fig. 1. Although some of bonding parameters are different in the indole and cyclohexyl rings of (I) and (II), these values are normal within their estimated standard deviations, as judged from the published values (Kennard, 1968). Selected torsion angles are listed in Table 2. The three rings in (I) are trigonally arranged, and the indole ring makes a dihedral angle of 34·0 (2) and 138·8 (2)° with the central and terminal cyclohexyl

Table 1. *Atomic coordinates for non-*H *atoms* (×10^4) *with their e.s.d.'s in parentheses*

	x	y	z	B_{eq}(Å^2)*
Compound (I)				
N(1)	10111 (3)	402 (1)	−1424 (2)	6·3
C(2)	9170 (4)	626 (1)	−621 (3)	5·7
C(3)	9617 (3)	1185 (1)	−169 (2)	4·7
C(4)	11864 (4)	1820 (2)	−633 (3)	6·6
C(5)	13047 (5)	1803 (3)	−1305 (4)	9·1
C(6)	13300 (5)	1300 (3)	−2057 (4)	9·7
C(7)	12411 (5)	801 (2)	−2172 (4)	8·5
C(8)	11203 (4)	811 (2)	−1482 (3)	5·9
C(9)	10916 (3)	1318 (1)	−714 (2)	4·9
C(10)	8901 (3)	1583 (1)	730 (3)	5·6
C(11)	9223 (3)	1390 (1)	2037 (2)	4·5
O(11)	9621 (3)	863 (1)	2316 (2)	6·4
N(12)	8995 (2)	1824 (1)	2896 (2)	3·8
C(13)	8333 (2)	2413 (1)	2597 (2)	3·7
O(13)	7066 (2)	2465 (1)	2517 (2)	5·7
N(14)	9224 (2)	2875 (1)	2460 (2)	4·1
C(15)	8763 (3)	3522 (1)	2287 (3)	4·7
C(16)	8517 (3)	3830 (1)	3505 (3)	6·2
C(17)	8106 (5)	5413 (2)	3324 (5)	8·5
C(18)	9204 (5)	4856 (2)	2632 (5)	9·1
C(19)	9465 (5)	4556 (2)	1442 (4)	8·5
C(20)	9880 (3)	3870 (1)	1602 (3)	5·9
C(21)	9103 (3)	1643 (1)	4190 (2)	4·3
C(22)	7739 (4)	1366 (2)	4588 (3)	6·3
C(23)	7838 (5)	1183 (2)	5923 (4)	8·5
C(24)	8312 (5)	1726 (2)	6711 (3)	8·2
C(25)	9680 (4)	1994 (2)	6318 (3)	7·3
C(26)	9560 (3)	2190 (2)	4996 (3)	5·9

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* Lists of structure factors, anisotropic thermal parameters for non-H atoms, coordinates and isotropic thermal parameters for H atoms, and hydrogen bonds and short contacts (<3·5 Å) have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38640 (35 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1 (*cont.*)

	x	y	z	B_{eq}(Å^2)*
Compound (II)				
Molecule *A*				
N(1)	8484 (7)	218 (5)	10612 (2)	4·2
C(2)	9285 (9)	1039 (6)	10423 (3)	4·1
C(3)	9665 (8)	1805 (6)	10769 (3)	3·8
C(4)	9100 (11)	1878 (8)	11652 (3)	5·3
C(5)	8359 (13)	1316 (8)	11979 (4)	6·4
C(6)	7629 (13)	339 (8)	11843 (4)	6·4
C(7)	7600 (10)	−94 (8)	11403 (4)	5·2
C(8)	8350 (9)	475 (7)	11080 (3)	4·1
C(9)	9092 (8)	1440 (6)	11198 (3)	3·7
C(10)	10477 (9)	2854 (6)	10737 (3)	3·8
C(11)	9748 (9)	3612 (7)	10343 (3)	4·4
N(12)	9905 (7)	3190 (5)	9861 (2)	4·1
C(13)	8756 (9)	2852 (6)	9541 (3)	3·5
O(13)	7446 (6)	3031 (4)	9582 (2)	4·0
N(14)	9191 (7)	2310 (6)	9165 (3)	4·5
C(15)	8112 (9)	1847 (7)	8791 (3)	4·7
C(16)	8788 (12)	1813 (8)	8318 (4)	6·1
C(17)	7694 (14)	1292 (9)	7916 (4)	7·6
C(18)	7334 (14)	168 (10)	8062 (4)	7·9
C(19)	6626 (12)	182 (8)	8528 (5)	7·1
C(20)	7679 (11)	682 (8)	8928 (4)	5·8
Molecule *B*				
N(1)	8011 (8)	4774 (5)	4387 (3)	4·7
C(2)	8976 (9)	3964 (6)	4580 (3)	4·2
C(3)	9087 (8)	3191 (7)	4247 (3)	4·0
C(4)	7830 (11)	3060 (8)	3353 (3)	5·4
C(5)	6815 (13)	3594 (9)	3021 (4)	6·7
C(6)	6187 (11)	4579 (9)	3132 (4)	6·4
C(7)	6518 (10)	5052 (7)	3582 (4)	5·1
C(8)	7520 (9)	4514 (7)	3917 (3)	4·2
C(9)	8196 (9)	3502 (6)	3809 (3)	4·2
C(10)	9978 (9)	2187 (7)	4302 (3)	4·1
C(11)	9534 (10)	1399 (7)	4686 (3)	4·6
N(12)	10053 (7)	1828 (6)	5166 (2)	4·3
C(13)	9171 (8)	2143 (6)	5474 (3)	3·8
O(13)	7790 (6)	1942 (4)	5417 (2)	4·4
N(14)	9795 (7)	2677 (6)	5866 (3)	4·7
C(15)	8936 (9)	3227 (7)	6198 (3)	4·2
C(16)	9851 (11)	3277 (8)	6699 (3)	5·8
C(17)	8961 (13)	3888 (10)	7042 (4)	7·2
C(18)	8599 (12)	5031 (8)	6864 (4)	6·6
C(19)	7693 (13)	4991 (9)	6370 (4)	6·9
C(20)	8517 (11)	4355 (7)	6023 (3)	5·3

* The B values are the equivalent isotropic temperature factors calculated from $B_{eq} = \frac{4}{3}(B_{11}a^2 + B_{22}b^2 + B_{33}c^2 + acB_{13}\cos\beta)$.

Table 2. *Selected torsion angles* (°)

Compound (I)	
C(2)–C(3)–C(10)–C(11)	83·8 (4)
C(9)–C(3)–C(10)–C(11)	−95·7 (3)
C(3)–C(10)–C(11)–N(12)	160·1 (2)
C(3)–C(10)–C(11)–O(11)	22·5 (4)
C(10)–C(11)–N(12)–C(13)	6·8 (3)
C(10)–C(11)–N(12)–C(21)	171·9 (2)
O(11)–C(11)–N(12)–C(13)	170·7 (7)
O(11)–C(11)–N(12)–C(21)	5·5 (4)
C(11)–N(12)–C(13)–N(14)	97·8 (3)
C(11)–N(12)–C(13)–O(13)	84·1 (3)
C(11)–N(12)–C(21)–C(22)	−84·5 (3)
C(11)–N(12)–C(21)–C(26)	150·8 (2)
C(21)–N(12)–C(13)–N(14)	96·8 (2)
C(21)–N(12)–C(13)–O(13)	−81·4 (3)
C(13)–N(12)–C(21)–C(22)	81·2 (3)
C(13)–N(12)–C(21)–C(26)	43·5 (3)
N(12)–C(13)–N(14)–C(15)	−173·2 (2)
O(13)–C(13)–N(14)–C(15)	4·9 (4)
C(13)–N(14)–C(15)–C(16)	84·0 (3)
C(13)–N(14)–C(15)–C(20)	−154·1 (2)

Compound (II)	*A*	*B*
C(2)–C(3)–C(10)–C(11)	57 (1)	62 (1)
C(9)–C(3)–C(10)–C(11)	−121·4 (9)	−118·9 (9)
C(3)–C(10)–C(11)–N(12)	−70·4 (9)	−73·9 (9)
C(10)–C(11)–N(12)–C(13)	113·7 (8)	114·6 (9)
C(11)–N(12)–C(13)–O(13)	13 (1)	12 (1)
C(11)–N(12)–C(13)–N(14)	−168·0 (7)	169·5 (8)
N(12)–C(13)–N(14)–C(15)	177·7 (7)	169·8 (8)
O(13)–C(13)–N(14)–C(15)	−3 (1)	12 (1)
C(13)–N(14)–C(15)–C(20)	−88·0 (9)	−85 (1)
C(13)–N(14)–C(15)–C(16)	151·7 (8)	153·4 (8)

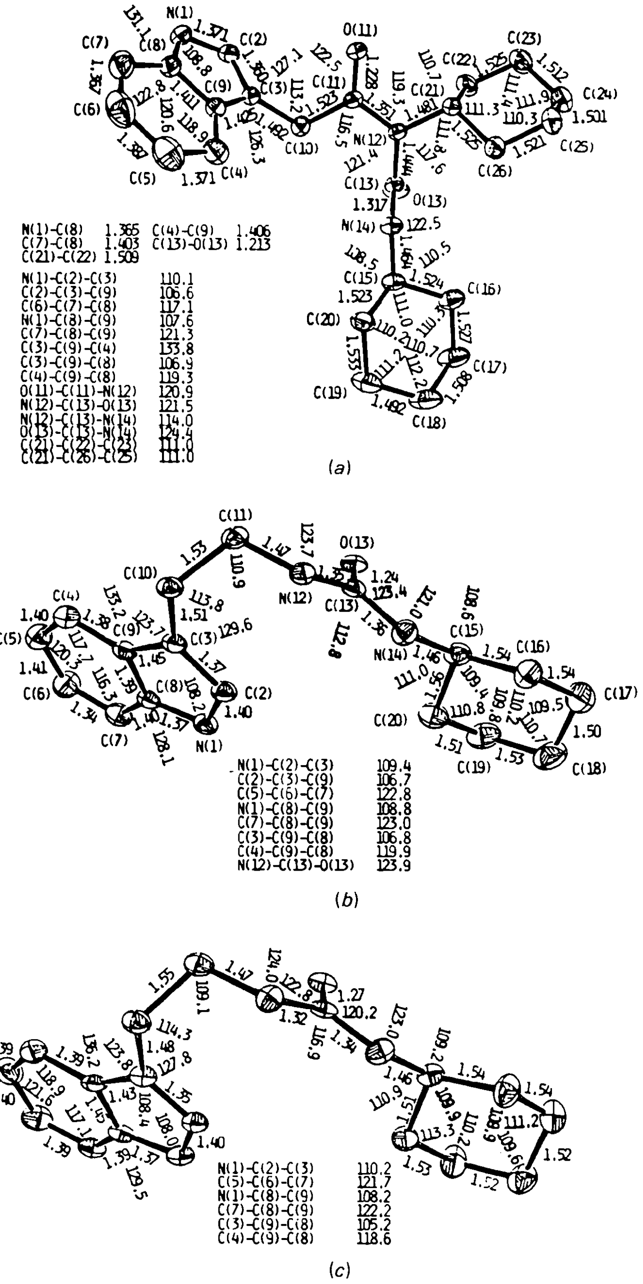

Fig. 1. Bond lengths (Å) and angles (°). (*a*) Compound (I); (*b*) and (*c*) molecules *A* and *B* of compound (II). The e.s.d.'s range from 0·003 to 0·008 Å (I) and 0·01 to 0·02 Å (II) for lengths, and from 0·2 to 0·5° (I) and 0·7 to 1·0° (II) for angles.

rings, respectively. On the other hand, the two crystallographically independent molecules *A* and *B* in (II) have almost the same extended conformations. The largest discrepancy between the molecules is in the torsion angle of O(13)—C(13)—N(14)—C(15): −3 (1) and −12 (1)° for *A* and *B*, respectively. The respective dihedral angles between the indole and cyclohexyl rings are 8·6 (5) and 12·8 (4)°.

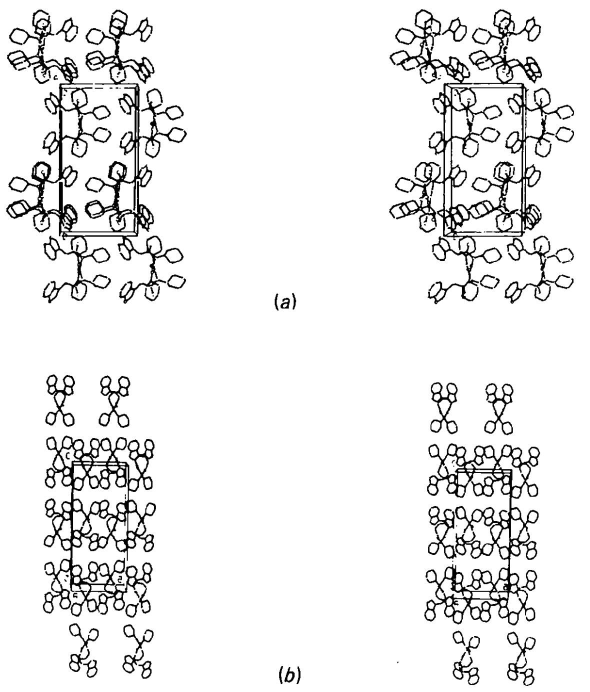

Fig. 2. Stereoscopic drawings of (*a*) (I) viewed along *a* axis, *b* axis vertical, *c* axis horizontal; and (*b*) (II) viewed along *a* axis, *c* axis vertical, *b* axis horizontal.

Fig. 2 shows the molecular packing of (I) and (II). In (I), the molecules related by *a*-glide symmetry form a molecular column with hexagonally arranged indole and cyclohexyl rings, and elongate parallel to the *a* axis. On the other hand, *A* and *B* in (II) form double layers consisting of indole and cyclohexyl rings perpendicular to the *c* axis. These layers in both crystals are stabilized by hydrogen-bond formation and van der Waals contacts with neighboring layers. Any specific interactions between the indole ring and the imide or urea group, which could account for the different spectral properties in their solution states, could not be observed in either crystal. The π-electron properties of the indole ring in (I) and (II) may be responsible for the difference, and are at present under consideration by molecular orbital methods.

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The Structure of Acetone Diethyl Sulfone,* $C_7H_{16}O_4S_2$, at 293 K and at 138 K

BY M. BILAYET HOSSAIN AND DICK VAN DER HELM

Department of Chemistry, University of Oklahoma, Norman, Oklahoma 73019, *USA*

AND A. K. ROY

Department of Physics, Dhaka University, Dhaka, Bangladesh

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Abstract. $M_r = 228{\cdot}3$, monoclinic, $P2/c$, $a = 17{\cdot}945\,(7)$, $b = 6{\cdot}229\,(1)$, $c = 19{\cdot}435\,(13)$ Å, $\beta = 90{\cdot}55\,(2)°$, $V = 2172{\cdot}3$ Å^3, $Z = 8$, $D_x = 1{\cdot}396$, $D_m = 1{\cdot}389$ g cm^{-3}, $\lambda(\mathrm{Cu}\,K\alpha) = 1{\cdot}54178$ Å, $\mu = 43{\cdot}2$ cm^{-1}, $F(000) = 976$, $R = 0{\cdot}067$ for 4460 diffractometer data ($2\theta_{\max} = 150°$), $T = 293$ K; $a = 17{\cdot}811\,(10)$, $b = 6{\cdot}121\,(2)$, $c = 19{\cdot}272\,(9)$ Å, $\beta = 90{\cdot}67\,(4)°$, $V = 2100{\cdot}9$ Å^3, $Z = 8$, $R = 0{\cdot}052$ for 4155 diffractometer data ($2\theta_{\max} = 150°$), $T = 138$ K. There is no significant difference between the room-temperature structure and the low-temperature structure. There are three different types of molecules in the unit cell. Two of these possess a twofold symmetry and their midpoints occupy special positions at ($x = 0$, $z = \frac{1}{4}$) and at ($x = \frac{1}{2}$, $z = \frac{1}{4}$). The center of the third molecule lies very close to ($x = \frac{1}{4}$, $z = 0$). Such packing gave rise to very strong pseudo orthorhombic symmetry for the crystal structure. Three molecules in the asymmetric unit are quite similar. The average S—C(ethyl) distance of 1·775 (1) Å is significantly shorter than the average of the other S—C bonds [1·829 (1) Å] in the molecule. The angular disposition of bonds around the S atoms in the present structure differs from those observed in other sulfones.

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* 2,2-Bis(ethylsulfonyl)propane.

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