crystal-structure-analysis package (Molecular Structure Corporation, 1985).

Related literature. The general procedure used in the synthesis of the title compound was originally employed by Tedjamulia, Tominaga, Castle & Lee (1983) in their preparation of 4-lithiodibenzothiophene. Utilizing their strategy various multisulfur-containing substituted dibenzothiophenes have been synthesized (Dunkerton, Barot & Nigam, 1987).

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Structure of Phenacyl Phenyl Sulfone

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Abstract. $C_{14}H_{12}O_3S$, $M_r = 260{\cdot}31$, monoclinic, $P2_1/c$, $a = 9{\cdot}231\,(3)$, $b = 5{\cdot}363\,(1)$, $c = 25{\cdot}742\,(10)$ Å, $\beta = 98{\cdot}49\,(3)°$, $V = 1260{\cdot}5\,(7)$ Å^3, $Z = 4$, $D_x = 1{\cdot}371$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 2{\cdot}07$ cm^{-1}, $F(000) = 544$, room temperature; final $R = 0{\cdot}039$ for 1086 observed reflections, $F(hkl) > 3{\cdot}92\sigma(F)$. Both benzene rings are planar within 0·03 Å. Five C—H bonds per molecule exhibit short contacts to O atoms: $d = 2{\cdot}41\,(4)$, 2·51 (5), 2·77 (4), 2·67 (4) and 2·55 (5) Å.

Experimental. Phenacyl phenyl sulfone (hereafter abbreviated to PPS) was obtained following Borchardt, Janota & Zakrzewski (1987). It was crystallized from ethanol yielding colourless needles. Monoclinic symmetry was estimated from oscillation and Weissenberg photographs. Density not measured. A crystal *ca* 0·6 × 0·2 × 0·15 mm was mounted on a Syntex $P2_1$ single-crystal diffractometer. Systematic absences: $h0l$, l odd, $0k0$, k odd, space group $P2_1/c$. Cell constants determined by the least-squares treatment of 15 reflections with 2θ values between 4·5 and 13·2°. Intensities collected at room temperature using graphite-monochromated Mo $K\alpha$ radiation up to $2\theta = 50°$, $-10 \leq h \leq 10$, $0 \leq k \leq 7$ and $0 \leq l \leq 31$, ω–2θ scan mode. 2135 independent intensities were collected, of which 165 were systematically absent. 1112 reflections classified as observed, $F_o > 3{\cdot}92\sigma(F_o)$. Correction for Lorentz and polarization effects but not for absorption. Two standard reflections, 2% intensity variation. The structure was solved using *MULTAN*80 (Main *et al.*, 1980) and refined by use of *SHELX*76 (Sheldrick, 1976). $\sum w(|F_o| - |F_c|)^2$ was minimized with $w = k/[\sigma^2(F_o) + GF_o^2]$ ($k = 1{\cdot}2266$, $G = 2{\cdot}609 \times 10^{-3}$). Atomic scattering factors supplied by *SHELX*76. E map gave positions of all non-H atoms ($R = 0{\cdot}45$). Location of H atoms and refinement of their positions led to final $R = 0{\cdot}039$, $wR = 0{\cdot}042$, $S = 1{\cdot}0138$; the final difference density map gave extreme values $-0{\cdot}31$ and $+0{\cdot}17$ e Å^{-3}; $(\Delta/\sigma)_{\max}$ in the last cycle 0·004 (mean 0·0009). Final positional parameters and equivalent isotropic temperature coefficients are given in Table 1.* Bond distances and bond angles are given in Table 2, the molecular structure and numbering of the atoms are shown in Fig. 1 [drawn with *PLUTO* (Motherwell, 1972)].

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51425 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Fractional coordinates* (× 10^4) *and equivalent isotropic temperature coefficients* (× 10^4) *for non*-H *atoms*

$$U_{eq} = (U_{11}U_{22}U_{33})^{1/3}.$$

	x	*y*	*z*	U_{eq}(Å^2)
S	5951 (1)	8029 (2)	776·2 (4)	43·1 (3)
O11	7014 (3)	6731 (5)	520 (1)	55 (1)
O12	5637 (3)	10597 (5)	642 (1)	56 (1)
O2	3319 (3)	5406 (6)	1420 (1)	66 (1)
C1	4288 (5)	6266 (9)	645 (2)	45 (2)
C2	3213 (4)	6715 (8)	1030 (1)	45 (1)
C11	6494 (4)	7884 (7)	1462 (1)	43 (1)
C12	5990 (5)	9648 (9)	1784 (2)	55 (2)
C13	6453 (6)	9540 (10)	2319 (2)	68 (2)
C14	7388 (6)	7710 (10)	2530 (2)	73 (2)
C15	7879 (7)	5980 (10)	2208 (2)	82 (2)
C16	7412 (5)	5999 (9)	1667 (2)	65 (2)
C21	2082 (4)	8687 (7)	921 (1)	43 (1)
C22	1045 (5)	8918 (9)	1267 (2)	59 (2)
C23	−14 (5)	10760 (10)	1182 (2)	70 (2)
C24	−68 (5)	12370 (10)	758 (2)	71 (2)
C25	949 (5)	12125 (9)	424 (2)	59 (2)
C26	2020 (4)	10321 (8)	500 (2)	49 (2)

Table 2. *Bond distances* (Å) *and valence angles* (°)

S–O11	1·439 (3)	S–O12	1·439 (3)
S–C1	1·792 (4)	S–C11	1·764 (4)
C1–C2	1·521 (5)	C2–C21	1·483 (5)
C2–O2	1·218 (4)		
C11–C12	1·383 (6)	C21–C22	1·406 (5)
C12–C13	1·381 (6)	C22–C23	1·384 (7)
C13–C14	1·364 (7)	C23–C24	1·386 (7)
C14–C15	1·369 (7)	C24–C25	1·370 (6)
C15–C16	1·394 (7)	C25–C26	1·376 (6)
C16–C11	1·374 (6)	C26–C21	1·388 (5)
O11–S–O12	118·7 (2)	S–C1–C2	114·7 (3)
O11–S–C1	106·3 (2)	C1–C2–C21	120·0 (4)
O11–S–C11	108·9 (2)	C1–C2–O2	117·7 (4)
O12–S–C1	108·9 (2)	O2–C2–C21	122·3 (3)
O12–S–C11	107·4 (2)		
C1–S–C11	105·9 (2)		
S–C11–C12	119·9 (3)	C2–C21–C22	118·0 (4)
S–C11–C16	119·1 (3)	C2–C21–C26	123·0 (4)
C16–C11–C12	121·0 (4)	C26–C21–C22	119·0 (4)
C11–C12–C13	119·1 (4)	C21–C22–C23	119·5 (5)
C12–C13–C14	120·9 (5)	C22–C23–C24	120·8 (5)
C13–C14–C15	119·5 (5)	C23–C24–C25	119·1 (5)
C14–C15–C16	121·2 (5)	C24–C25–C26	121·4 (5)
C15–C16–C11	118·2 (5)	C25–C26–C21	120·1 (4)

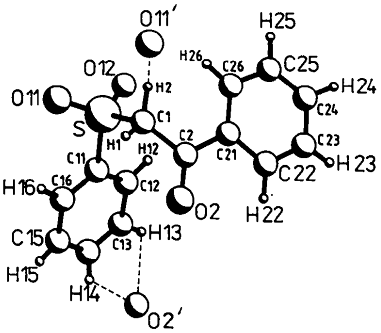

Fig. 1. The phenacyl phenyl sulfone molecule with labelling and three of the shortest H···O contacts.

Related literature. Phenacyl phenyl sulfone is an example of a system with acidic C—H bonds. Amel & Marek (1973) have studied acid/base equilibria in derivatives substituted in the phenyl part of the PPS molecule and found the Hammett equation to be held. Borchardt, Kornacki, Kopkowski & Zakrzewski (1988) have found that proton NMR chemical shifts of this CH_2 group follow the same rule.

Analysis of benzene-ring geometry leads to the conclusion that the bond angles and distances within both benzene rings seem normal. The bond angle at the substituted carbon is slightly greater than 120° (*i.e.* 121·0°) due to the high electronegativity of the SO_2 group. Differences between the observed angles and those predicted by the additivity rule by use of angular substituent parameters (Norrestam & Schepper, 1978, 1981; Domenicano & Murray-Rust, 1979) are not significant.

Both rings are planar within 0·03 Å. The sulfone-group and carbonyl-group geometries are normal.

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