The $^+S-C^-$ distance of 1·689 (3) Å is statistically shorter than that observed in the sulfonium ylides series [1·715 (4) to 1·743 (4) Å], but it is equivalent to the 1·688 (3) Å value found in TBO. The two $^+S-C(sp^2)$ distances of 1·760 (4) and 1·768 (4) Å are equivalent to those reported in the sulfonium ylide series and to those in TBO. The ^+S-O distance of 1·445 (3) Å is statistically shorter than the 1·458 (3) Å value found in TBO but is equivalent to the mean value of 1·440 (2) Å found in thioxanthene 10,10 dioxide (Chu & Chung, 1974) and 9-isobutylthioxanthene 10,10-dioxide (Chu & Chung, 1973). The C—C distances around the phenyl rings average 1·389 (6) Å [1·373 (8) to 1·400 (6) Å] while the distances and angles associated with the carbanion moiety are internally consistent and equivalent to those in reference compounds cited above.

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N^1-Phenylsulphanilamide, $C_{12}H_{12}N_2O_2S$*

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Abstract. $M_r = 248·3$, orthorhombic, *Pcab* [nonstandard setting of *Pbca*, equivalent positions $\pm(x,y,z;$ $\frac{1}{2}-x,y, \frac{1}{2}+z; \frac{1}{2}+x, \frac{1}{2}-y,z; x, \frac{1}{2}+y, \frac{1}{2}-z)$], $a = 24·230$ (8), $b = 15·500$ (5), $c = 6·034$ (2) Å, $V = 2266·16$ Å^3, $Z = 8$, $D_m = 1·460$ (5), $D_x = 1·455$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0·71069$ Å, $\mu = 0·137$ mm^{-1}, $F(000) = 1040$, room temperature, $R = 0·035$ for 814 reflexions [$I > 3\sigma(I)$]. The molecules are linked along **b** by a system of three hydrogen bonds N—H···O per molecule through the unsubstituted amino group. Apart from an appreciable quinonoid character in the aniline ring caused by proton transfer on nitrogen, bond lengths and inter-bond angles have standard values.

Introduction. This work was undertaken as part of a programme relating the crystal structures of various sulpha compounds (Cook & Turner, 1975, 1976) to their therapeutic activity in the treatment of infections in burns. The material was supplied by Messrs Smith & Nephew Limited, Harlow.

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* Sulphanilanilide.

Table 1. *Final atomic parameters and e.s.d.'s*

$$B_{eq} = \tfrac{4}{3} \left(\frac{\beta_{11}}{a^{*2}} + \frac{\beta_{22}}{b^{*2}} + \frac{\beta_{33}}{c^{*2}} \right).$$

	x	y	z	$B_{eq}(\text{Å}^2)$
S	0·1635 (1)	0·4073 (1)	0·1778 (2)	4·66 (2)
O(1)	0·1471 (1)	0·3990 (2)	0·4067 (7)	7·04 (8)
O(2)	0·2109 (1)	0·4565 (2)	0·1123 (6)	6·12 (7)
N(1)	0·1104 (1)	0·4559 (2)	0·0564 (5)	3·51 (6)
N(2)	0·1855 (1)	0·0565 (2)	−0·1878 (6)	5·98 (8)
C(1)	0·0575 (2)	0·4176 (3)	0·0578 (10)	6·00 (10)
C(2)	0·0256 (2)	0·4282 (3)	0·2466 (9)	4·99 (8)
C(3)	−0·0275 (2)	0·3941 (2)	0·2778 (8)	4·39 (8)
C(4)	−0·0479 (2)	0·3469 (4)	0·0954 (9)	7·27 (12)
C(5)	−0·0134 (2)	0·3313 (4)	−0·0872 (10)	7·46 (13)
C(6)	0·0395 (2)	0·3647 (2)	−0·1081 (6)	3·97 (7)
C(7)	0·1712 (1)	0·3031 (2)	0·0598 (5)	2·48 (6)
C(8)	0·1962 (1)	0·2882 (3)	−0·1403 (7)	4·62 (8)
C(9)	0·1977 (1)	0·2072 (2)	−0·2219 (7)	3·63 (6)
C(10)	0·1770 (2)	0·1374 (3)	−0·0989 (9)	5·20 (9)
C(11)	0·1526 (1)	0·1525 (2)	0·1087 (6)	3·36 (6)
C(12)	0·1496 (2)	0·2346 (3)	0·1830 (7)	5·40 (10)

Table 2. *Bond lengths (Å) and inter-bond angles (°)*

S—O(1)	1·443 (4)	C(5)—C(6)	1·389 (7)
S—O(2)	1·435 (4)	C(6)—C(1)	1·366 (7)
S—N(1)	1·661 (3)	C(7)—C(8)	1·370 (6)
S—C(7)	1·775 (4)	C(8)—C(9)	1·349 (6)
N(1)—C(1)	1·411 (5)	C(9)—C(10)	1·404 (6)
C(1)—C(2)	1·387 (8)	C(10)—N(2)	1·379 (6)
C(2)—C(3)	1·403 (6)	C(10)—C(11)	1·406 (6)
C(3)—C(4)	1·410 (7)	C(11)—C(12)	1·352 (6)
C(4)—C(5)	1·404 (8)	C(12)—C(7)	1·398 (6)
O(1)—S—O(2)	122·1 (2)	C(4)—C(5)—C(6)	123·8 (5)
O(1)—S—N(1)	104·4 (2)	C(1)—C(6)—C(5)	116·8 (4)
O(1)—S—C(7)	109·4 (2)	S—C(7)—C(8)	123·6 (3)
O(2)—S—N(1)	105·0 (2)	S—C(7)—C(12)	116·0 (3)
O(2)—S—C(7)	106·8 (2)	C(8)—C(7)—C(12)	120·4 (4)
N(1)—S—C(7)	108·5 (2)	C(7)—C(8)—C(9)	119·4 (4)
S—N(1)—C(1)	120·7 (3)	C(8)—C(9)—C(10)	121·0 (4)
N(1)—C(1)—C(2)	117·5 (4)	C(9)—C(10)—C(11)	119·6 (4)
N(1)—C(1)—C(6)	122·5 (4)	N(2)—C(10)—C(9)	116·2 (4)
C(2)—C(1)—C(6)	119·7 (5)	N(2)—C(10)—C(11)	124·1 (4)
C(1)—C(2)—C(3)	125·2 (4)	C(10)—C(11)—C(12)	118·3 (4)
C(2)—C(3)—C(4)	114·3 (4)	C(7)—C(12)—C(11)	121·3 (4)
C(3)—C(4)—C(5)	119·6 (5)		

Experimental. Crystals prepared by slow evaporation of 10% ammonia solution at room temperature in the dark; acicular crystals *ca* $1\cdot0 \times 0\cdot2 \times 0\cdot2$ mm, D_m by flotation in NaI solution, analysis: C 58·1, H 4·8, N 11·3, S 12·9%, required for $C_{12}H_{12}N_2O_2S$: C 58·0, H 4·9, N 11·3, S 12·9%, m.p. 470 (1) K, lattice parameters initially from rotation and Weissenberg photographs but subsequently refined on Stoe Stadi-2 Weissenberg-geometry diffractometer by least-squares fits to the 2θ angles of 14 reflexions, intensities measured with ω scans, crystal mounted about c, $2\theta_{max} = 50°$, index range h 0–28, k 0–18, l 0–5; 6 standard reflexions, no variation; 1547 independent reflexions, 733 with $I < 3\sigma(I)$, corrections for Lp not for absorption; structure solved with *SHELX* (Sheldrick, 1976) and *MULTAN* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), refinement by least squares on F using *NRC* programs (Ahmed, Hall,

Pippy & Huber, 1970) on our DEC-10 computer, H coordinates of atoms bonded to the two rings calculated, those bonded to amino N found from Fourier difference map; H parameters used in F calculations with $B_{iso} = 6\cdot0$ Å^2, not refined, other atoms refined with B_{iso} initially and finally B_{ij} until in last cycle all shifts $<0\cdot3\sigma$, residual $\Delta\rho$ in final difference synthesis within $\pm0\cdot1$ e Å^{-3}, scattering factors from *International Tables for X-ray Crystallography* (1962), $R = 0\cdot035$, $wR = 0\cdot061$, $w^{1/2} = 1/F_o$.

Discussion. Atomic coordinates and equivalent isotropic temperature factors are given in Table 1,* and bond lengths and inter-bond angles in Table 2. Molecules are linked along **b** by a system of three H bonds per molecule, N(2)···O(2'), N(2)···O(2'') and N(2)···O(1''') with mean length 3·052 (4) Å, as shown in Fig. 1. This implies that N(2) has three H atoms bonded to it while N(1), as confirmed by a difference synthesis, has none; proton transfer has taken place and this also results in a pronounced quinonoid character of the aniline ring; C(8)—C(9) and C(11)—C(12) are nearly double bonds ($\sim1\cdot35$ Å) while C(7)—C(12), C(9)—C(10) and C(10)—C(11) are $\sim1\cdot40$ Å.

* Lists of structure factors, anisotropic temperature factors, calculated H-atom parameters and results of mean-plane calculations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39173 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
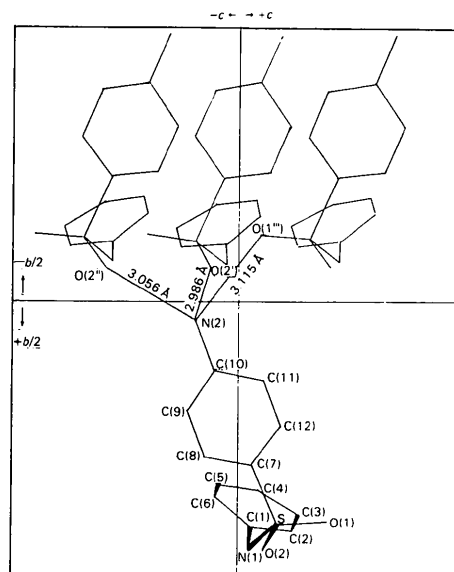

Fig. 1. Projection of molecules on (100) showing numbering of atoms and H-bonding distances (e.s.d.'s are 0·005 Å). Symmetry code: (i) $\tfrac{1}{2} - x, y - \tfrac{1}{2}, -z$; (ii) $x, y - \tfrac{1}{2}, -\tfrac{1}{2} - z$; (iii) $x, y - \tfrac{1}{2}, \tfrac{1}{2} - z$.

There is a noticeable shortening effect for one bond in each ring, *i.e.* C(7)—C(8) 1·370 (6) and C(1)—C(6) 1·366 (7) Å; no explanation can be offered for this, but exactly the same effect was observed in the 2-chloro derivative (Shefter, 1976) where the two bonds are 1·376 and 1·361 Å, respectively. S—C(7) at 1·775 (4) Å agrees with 1·766 Å found in sodium naphthionate tetrahydrate (Brown & Corbridge, 1966) and S—N(1) at 1·661 (3) Å agrees with 1·666 Å in γ-sulphanilamide (Alléaume & Decap, 1965). The other bonds in the molecule are similar to those found in other sulphanilamides and sulphadiazines; a table of comparisons is given by Cook & Turner (1975).

The two rings are effectively planar, for C(1)—(6) the r.m.s. deviation is 0·030 (5) Å and for C(7)—(12) 0·012 (4) Å. The dihedral angle between them is 50·65 (5)°.

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Structure of 1-Diphenylmethyl-3-hydroxyazetidinium Chloride,* $C_{16}H_{18}NO^+.Cl^-$

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Abstract. $M_r = 275\cdot8$, monoclinic, $P2_1/a$, $a = 12\cdot356$ (5), $b = 9\cdot054$ (4), $c = 14\cdot043$ (4) Å, $\beta = 100\cdot34$ (3)°, $V = 1545\cdot5$ Å^3, $Z = 4$, $D_m = 1\cdot14$, $D_x = 1\cdot185$ Mg m^{-3}, μ(Mo $K\alpha$, $\lambda = 0\cdot7107$ Å) = 2·77 mm^{-1}, $F(000) = 584\cdot0$, $T = 293$ K, $R = 0\cdot053$ for 1088 reflections. The four-membered ring is buckled 13·0° ($\theta = 167\cdot0$°). The azetidinium moiety is linked to the Cl$^-$ ion through a hydrogen bond [O—H···Cl = 3·166 (5) Å].

Introduction. Structural studies on compounds containing the azetidine ring are important for the interpretation of their stereochemical and biological significance. In this connection our findings on the molecular geometry of the title compound (DPHA) are presented. The samples of DPHA were provided by Dr Joseph John of the Department of Science and Technology, India.

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Experimental. Small, pale-yellow needles (from acetone solution). D_m by flotation in bromoform/benzene. Crystal 0·38 × 0·25 × 0·5 mm. Enraf–Nonius CAD-4/11M single-crystal X-ray diffractometer. Lattice parameters from 20 reflections ($12° < 2\theta < 26°$). Data collection: h, k, $\pm l$ with $2\theta \le 48°$; Mo $K\alpha$ radiation, graphite monochromator; $\omega/2\theta$ scan mode. Three standard reflections every 2000 s: no significant variation. 2707 independent reflections, 1088 with $F > 3\sigma(F)$. Lp correction. No absorption or decay corrections. $P2_1/a$, general positions $\pm(x, y, z; \frac{1}{2}-x, \frac{1}{2}+y, -z)$, from systematic absences 0k0, $k \ne 2n$ and h0l, $h \ne 2n$. Direct methods (*MULTAN*78; Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). Anisotropic full-matrix refinement for non-H atoms (*LALS*; Gantzel, Sparks & Trueblood, 1961). H from stereochemical considerations and verified from ΔF synthesis, only positions refined, $R = 0\cdot053$, $R_w = 0\cdot057$; $\sum w(|F_o| - |F_c|)^2$ minimized, where $w = 1/(a + bF + cF^2)$ with $a = 3\cdot5$, $b = 1\cdot0$ and $c = 0\cdot025$. $(\Delta/\sigma)_{max} = 0\cdot01$. Final $\Delta\rho$ map featureless. No correction for