Table 1. *Final atomic coordinates and equivalent isotropic temperature factors*

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq} (Å^2)
N(1)	−0·0823 (6)	0·6200 (1)	0·4468 (2)	3·99 (6)
C(2)	0·0653 (7)	0·6367 (1)	0·3446 (2)	3·45 (7)
C(3)	0·1409 (9)	0·6088 (1)	0·2392 (3)	4·49 (8)
C(4)	0·0471 (10)	0·5590 (1)	0·2421 (3)	5·16 (10)
C(5)	−0·1059 (9)	0·5406 (1)	0·3480 (3)	4·80 (9)
C(6)	−0·1656 (9)	0·5717 (1)	0·4464 (3)	4·72 (9)
O(7)	0·1719 (6)	0·6863 (1)	0·3554 (2)	4·16 (5)
C(8)	0·0839 (7)	0·7194 (1)	0·2655 (2)	3·19 (6)
O(8)	−0·0950 (6)	0·7093 (1)	0·1765 (2)	4·50 (6)
C(9)	0·2272 (6)	0·7695 (1)	0·2921 (2)	2·95 (6)
C(10)	0·3980 (7)	0·7804 (1)	0·4045 (2)	3·17 (6)
C(11)	0·5183 (7)	0·8279 (1)	0·4270 (2)	3·17 (6)
N(12)	0·5997 (7)	0·9140 (1)	0·3580 (2)	4·42 (7)
C(12)	0·4670 (7)	0·8636 (1)	0·3355 (2)	3·20 (6)
C(13)	0·3002 (7)	0·8536 (1)	0·2228 (2)	3·49 (7)
C(14)	0·1786 (7)	0·8062 (1)	0·2027 (2)	3·29 (6)
O(1)	0·7364 (9)	0·9229 (1)	0·4575 (2)	7·58 (9)
O(2)	0·5736 (9)	0·9443 (1)	0·2749 (2)	7·20 (9)

Table 2. *Selected bond lengths* (Å) *and valency and torsional angles* (°)

C(2)—O(7)	1·402 (3)	N(12)—O(1)	1·206 (3)
C(8)—O(7)	1·350 (3)	N(12)—O(2)	1·207 (3)
C(8)—O(8)	1·202 (3)	N(1)—C(2)	1·309 (3)
C(8)—C(9)	1·485 (4)	N(1)—C(6)	1·339 (4)
C(12)—N(12)	1·470 (4)		
C(2)—O(7)—C(8)	119·8 (2)	C(12)—N(12)—O(2)	118·4 (2)
O(7)—C(8)—O(8)	123·5 (3)	O(1)—N(12)—O(2)	123·0 (3)
O(7)—C(8)—C(9)	111·8 (2)	C(2)—N(1)—C(6)	115·9 (2)
O(8)—C(8)—C(9)	124·7 (2)	N(1)—C(2)—C(3)	125·5 (3)
C(12)—N(12)—O(1)	118·6 (2)		
N(1)—C(2)—O(7)—C(8)	−129·9 (3)	O(7)—C(8)—C(9)—C(10)	−6·4 (3)
C(3)—C(2)—O(7)—C(8)	55·3 (4)	O(8)—C(8)—C(9)—C(14)	−6·2 (4)
C(2)—O(7)—C(8)—O(8)	2·8 (4)	O(1)—N(12)—C(12)—C(11)	−2·9 (4)
C(2)—O(7)—C(8)—C(9)	−178·7 (2)	O(2)—N(12)—C(12)—C(13)	−3·6 (4)

Related literature. 2-Chloro-4,6-disubstituted-1,3,5-triazines have lately been proposed as a very efficient activator of the carboxylic group in the syntheses of esters, amides, carboxylic acid anhydrides and peptides (Kamiński, 1985, 1987). A comparison of an intermediate product, 2-(2,2-dimethylpropanoyloxy)-4,6-dimethoxy-1,3,5-triazine, with its benzene analog, the 4-nitrophenyl ester of 2,2-dimethylpropanoic acid, has shown that enhanced reactivity of the former substrate in the acylation reaction (Kamiński, Główka & Iwanicka, 1989) may result either from favourable electronic factors or from stabilization of a cyclic intermediate in the *s*-triazine derivative (Główka, Iwanicka & Kamiński, 1990). The present results are in agreement with this interpretation.

In the crystal, the molecules are packed almost perpendicular to the [100] direction. The angle between (100) and the pyridine least-squares plane is about 26° (29° for the benzene least-squares plane) and the distances between parallel rings are 3·47 Å (pyridine) and 3·38 Å (benzene).

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Structure of *p*-Chlorobenzenesulfonic Acid Monohydrate

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Abstract. Oxonium *p*-chlorobenzenesulfonate, $C_6H_4ClO_3S^-.H_3O^+$, $M_r = 210{\cdot}6$, monoclinic, $P2_1/c$, $a = 6{\cdot}000\,(1)$, $b = 7{\cdot}250\,(1)$, $c = 19{\cdot}696\,(4)$ Å, $\beta = 98{\cdot}17\,(2)°$, $V = 848{\cdot}1\,(1)$ Å^3, $Z = 4$, $D_m = 1{\cdot}65$, $D_x = 1{\cdot}649$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 6{\cdot}55$ cm^{-1}, $F(000) = 432$, $T = 296$ K, $R = 0{\cdot}036$ for 2241 unique observed reflections. The average S—O, C—S—O and O—S—O values are 1·453 (2) Å,

105·97 (5) and 112·77 (5)°, respectively. The pyramidal H_3O^+ ion forms three hydrogen bonds of 2·555 (3), 2·569 (3) and 2·560 (3) Å to the O atoms of different sulfonate groups.

Experimental. A colorless crystal (0·3 × 0·3 × 0·4 mm) obtained from aqueous solution was mounted on a Rigaku AFC-5RU diffractometer. Density measured by flotation. Cell dimensions were determined by a least-squares method to the setting angles of 20 reflections having $13 < \theta < 17°$. Intensity data of 2555 reflections ($0 \leq h \leq 8$, $0 \leq k \leq 10$, $-27 \leq l \leq 27$) were collected within a range of $2\theta < 60°$, using graphite-monochromated Mo $K\alpha$ radiation; 2θ–ω scans at speeds of 2° min^{-1} were made over a range of $(1{\cdot}0 + 0{\cdot}5\tan\theta)°$. Three standard reflections showed no significant fluctuation during data collection. Data were corrected for Lorentz and polarization factors, but no absorption correction was applied. Structure was solved with *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), and refined by full-matrix least squares based upon F with $w = [\sigma^2(F_o) + (0{\cdot}023F)^2]^{-1}$. Non-H atoms were refined anisotropically. H atoms were located by difference Fourier synthesis, and refined isotropically. Atomic scattering factors used were obtained from *International Tables for X-ray Crystallography* (1974). The final R value was 0·036 ($wR = 0{\cdot}060$, $S = 1{\cdot}7$) for 2241 unique reflections with $F_o > 3\sigma$; parameter shifts were less than $0{\cdot}2\sigma$, and maximum residual density was 0·25 e Å^{-3}.

All computations were performed on a FACOM M780 computer in the Data Processing Center of Kyoto University, using the program *KPPXRAY* (Taga, Higashi & Iizuka, 1985).

The molecular structure with the labeling scheme is shown in Fig. 1. The atomic parameters are listed in Table 1. Bond distances and angles are listed in Table 2.*

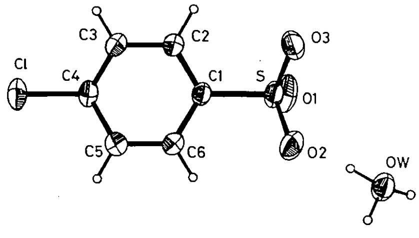

Fig. 1. A view of the *p*-chlorobenzenesulfonate anion and H_3O^+ cation with the atomic numbering and thermal ellipsoids drawn at the 50% probability level.

Table 1. *Atomic coordinates and equivalent isotropic temperature factors*

$$B_{eq} = (4/3)\textstyle\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}(Å^2)
S	0·3076 (1)	0·1567 (1)	0·11081 (2)	2·81 (1)
Cl	0·2516 (1)	0·1878 (1)	0·42431 (2)	4·14 (2)
O(1)	0·2145 (3)	−0·0233 (2)	0·0900 (1)	4·51 (6)
O(2)	0·5440 (2)	0·1744 (2)	0·1037 (1)	4·47 (7)
O(3)	0·1710 (2)	0·3068 (2)	0·0784 (1)	3·51 (5)
O(*W*)	0·7828 (2)	0·2507 (2)	0·0090 (1)	3·44 (5)
C(1)	0·2930 (2)	0·1723 (2)	0·1993 (1)	2·30 (5)
C(2)	0·0993 (3)	0·2385 (3)	0·2218 (1)	2·81 (5)
C(3)	0·0865 (3)	0·2454 (3)	0·2916 (1)	2·93 (6)
C(4)	0·2680 (3)	0·1851 (2)	0·3375 (1)	2·65 (5)
C(5)	0·4631 (3)	0·1197 (3)	0·3155 (1)	3·03 (6)
C(6)	0·4756 (3)	0·1136 (2)	0·2460 (1)	2·77 (6)

Table 2. *Bond distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

S—O(1)	1·455 (2)	S—O(2)	1·451 (1)
S—O(3)	1·454 (1)	S—C(1)	1·761 (2)
Cl—C(4)	1·727 (2)	C(1)—C(2)	1·387 (2)
C(1)—C(6)	1·393 (2)	C(2)—C(3)	1·389 (2)
C(3)—C(4)	1·384 (2)	C(4)—C(5)	1·388 (2)
C(5)—C(6)	1·382 (2)		
O(1)—S—O(2)	113·2 (1)	O(1)—S—O(3)	112·2 (1)
O(1)—S—C(1)	105·4 (1)	O(2)—S—O(3)	112·9 (1)
O(2)—S—C(1)	106·1 (1)	O(3)—S—C(1)	106·4 (1)
S—C(1)—C(2)	120·0 (1)	S—C(1)—C(6)	119·3 (1)
C(2)—C(1)—C(6)	120·7 (1)	C(1)—C(2)—C(3)	119·7 (1)
C(2)—C(3)—C(4)	119·1 (2)	Cl—C(4)—C(3)	119·5 (1)
Cl—C(4)—C(5)	118·8 (1)	C(3)—C(4)—C(5)	121·6 (1)
C(4)—C(5)—C(6)	119·1 (1)	C(1)—C(6)—C(5)	119·7 (1)

Related literature. The structure of an isomorphous monoclinic crystal, *p*-toluenesulfonic acid monohydrate, has been reported by Arora & Sundaralingam (1971), and its neutron study to determine the accurate hydrogen positions around the oxonium ion has been reported by Lundgren & Williams (1973). Another modification of *p*-toluenesulfonic acid monohydrate (orthorhombic form) has been determined by Dexter (1971).

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* Lists of atomic parameters for H atoms, anisotropic thermal parameters for non-H atoms and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52699 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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