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Structure of Sulfisomidine Dihydrochloride Dihydrate

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Abstract. 4-Amino-*N*-(2,6-dimethyl-4-pyrimidinyl)-benzenesulfonamide dihydrochloride dihydrate, $C_{12}H_{16}N_4O_2S^{2+}.2Cl^-.2H_2O$, $M_r = 387{\cdot}3$, triclinic, $P\bar{1}$, $a = 13{\cdot}400\,(4)$, $b = 14{\cdot}474\,(3)$, $c = 5{\cdot}091\,(2)$ Å, $\alpha = 99{\cdot}73\,(2)$, $\beta = 94{\cdot}82\,(3)$, $\gamma = 111{\cdot}42\,(2)°$, $V = 894{\cdot}5$ Å^3, $Z = 2$, $D_x = 1{\cdot}44$ g cm^{-3}, $\lambda(\mathrm{Cu}\,K\alpha) = 1{\cdot}5418$ Å, $\mu = 45{\cdot}153$ cm^{-1}, $F(000) = 404$, $T = 277\,(1)$ K, $R = 0{\cdot}040$, $wR = 0{\cdot}051$ for 1670 observed reflections. The conformation of the compound is similar to that observed in other sulfonamides. The

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dihedral angle between the benzene and pyrimidine rings is 78·6 (5)°. The arrangement of atoms around the sulfur atom is distorted from ideal tetrahedral geometry, angular range 102·9 (2)–120·5 (2)°. The crystal structure is stabilized by an intricate network of hydrogen bonds.

Introduction. Sulfisomidine is a rapidly absorbed and rapidly excreted sulfonamide that is acetylated to only a small degree and has been used extensively for the treatment of urinary tract infections (Weinstein, 1966). In order to study the influence on the hydrogen-bonding pattern and on the molecular structure and conformation of sulfonamides on forming a halide derivative, we report here the crystal structure of sulfisomidine dihydrochloride dihydrate and compare the structural parameters with those of sulfisomidine base previously determined by Singh, Tiwari & Singh (1985).

Experimental. Crystallized from commercially available sulfisomidine dissolved in an excess amount of dilute HCl, crystal size 0·20 × 0·15 × 0·10 mm. Syntex $P\bar{1}$ diffractometer, graphite-monochromated Cu $K\alpha$ radiation, cell dimensions from setting angles of 15 reflections in the range $45° < 2\theta < 67°$, no systematic absences, space group $P\bar{1}$ confirmed by successful refinement. ω–2θ scans, 1686 independent reflections, $2\theta \leq 120°$, index range h 0 to 14, k −15 to 14, l −5 to 5, 1670 observed with $I > 2\sigma(I)$; three standard reflections, measured after every 97 reflections; no significant intensity variation, no absorption correction. Structure solved by *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978); H atoms located from difference Fourier map: non-H atoms refined anisotropically, H atoms isotropically, least-squares refinement, $\sum w(\Delta F)^2$ minimized, $w = 1/\sigma^2(F)$, $R = 0·040$, $wR = 0·051$, $S = 1·49$, highest parameter shift-to-error ratio 0·70, $\Delta\rho$ in final difference Fourier map within ±0·38 e Å^{-3}, scattering factors from *International Tables for X-ray Crystallography* (1974), *XRAY ARC* (1971) program system used for most of the calculations.

Table 1. *Fractional atomic coordinates* (× 10^4) *with e.s.d.'s in parentheses and equivalent isotropic temperature factors* (Å^2) *for non-hydrogen atoms*

$$B_{eq} = \tfrac{4}{3}\sum_i\sum_j \mathbf{a}_i.\mathbf{a}_j\beta_{ij}.$$

	x	y	z	B_{eq}
Cl(1)	6732 (1)	9231 (1)	4340 (2)	3·72
Cl(2)	3657 (1)	6035 (1)	3026 (2)	4·20
S	9509 (1)	1936 (1)	5622 (2)	2·67
O(1)	9590 (2)	2898 (2)	5072 (5)	3·10
O(2)	9455 (2)	1133 (2)	3506 (5)	3·54
N(1)	13314 (2)	2753 (2)	13874 (6)	3·20
N(2)	8386 (2)	1426 (2)	6884 (6)	3·00
N(3)	8475 (2)	2911 (2)	9701 (6)	2·74
N(4)	7200 (2)	2803 (2)	12603 (6)	2·69
C(1)	12327 (3)	2534 (2)	11993 (7)	2·68
C(2)	11959 (3)	3293 (2)	11782 (9)	3·75
C(3)	11078 (3)	3099 (3)	9901 (9)	3·40
C(4)	10576 (3)	2151 (2)	8194 (7)	2·38
C(5)	10937 (3)	1385 (3)	8490 (8)	3·38
C(6)	11811 (3)	1579 (2)	10373 (8)	3·24
C(7)	7981 (3)	1895 (2)	8845 (7)	2·40
C(8)	7094 (3)	1303 (2)	9872 (7)	2·85
C(9)	6691 (3)	1773 (2)	11793 (7)	2·55
C(10)	8069 (3)	3340 (2)	11589 (7)	2·78
C(11)	8581 (3)	4461 (3)	12659 (10)	4·47
C(12)	5749 (3)	1250 (3)	13080 (8)	3·43
O(*W*1)	4644 (2)	2676 (2)	160 (6)	5·92
O(*W*2)	6135 (3)	5339 (2)	2662 (7)	6·15

Discussion. Atomic coordinates are listed in Table 1;* bond lengths, bond angles and selected torsion angles are in Table 2. An *ORTEP* drawing (Johnson, 1965) of the molecule with the atomic numbering is shown in Fig. 1. The average C—H, N—H and O—H distances in the molecule are 0·93 (4), 0·90 (4) and 0·82 (6) Å, respectively. The principal structural differences observed between sulfisomidine dihydrochloride dihydrate and sulfisomidine base (Singh *et al.*, 1985) are: (i) quinoidal character of the phenyl ring in the present structure; (ii) the S—N(2)—C(7) angle is 127·8 (2)°, compared with 120·4 (2)° in sulfisomidine base; (iii) the pyrimidine ring is planar, while it is folded in sulfisomidine base.

It has been suggested (Kumler & Halverstadt, 1941; Kumler & Strait, 1943; Shefter, Chmielewicz, Blount, Brennan, Sackman & Sackman, 1972) that the ability of the sulfanilamide portion of these molecules to form the resonance quinoid structure might influence their activity. In the present structure the phenyl ring has a small amount of quinoidal character, *i.e.* the C(2)—C(3) and C(5)—C(6) bonds are slightly shorter than the four other phenyl ring bonds. A similar situation has also been observed in sulfamerazine (Acharya, Kuchela & Kartha, 1982), and sulfadimethoxine and sulfadoxine (Shefter *et al.*, 1972). The bond lengths in the pyrimidine ring vary from 1·318 (4) to 1·390 (5) Å and the bond angles from 116·6 (3) to 123·2 (3)°. These parameters are in accord with those observed in some other sulfonamides having a pyrimidine ring. The phenyl ring is planar to within +0·018 (3) and −0·012 (4) Å, while the pyrimidine ring is planar to within ±0·007 (3) Å. The methyl C(11) and C(12) atoms are displaced by −0·030 (5) and −0·008 (4) Å from the pyrimidine plane.

The coordination around the S atom is distorted from ideal tetrahedral geometry. The largest deviation is in the angle O(1)—S—O(2), 120·5 (2)°, while the other

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* Lists of structure amplitudes, anisotropic thermal parameters, H-atom parameters and least-squares-planes calculations have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43092 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

angles are in the range 102·9 (2)–109·8 (2)°. This distorted arrangement has been observed in most of the sulfonamides (Chatterjee, Dattagupta & Saha, 1981).

The S—N(2)—C(7) angle [127·8 (2)°] is large compared with the corresponding angle in sulfisomidine base [120·4 (2)°]. A large angle has also been found in a number of substituted sulfonamides, *e.g.* 125·9° in sulfadimethoxine, 126·7° in sulfadoxine (Shefter *et al.*, 1972); 128·1° in sulfamerazine (Acharya *et al.*, 1982) and 126·0° in sulfadimidine (Tiwari, Haridas & Singh, 1984). The conformation of the sulfonamide grouping is similar to that in related molecules. Earlier studies (Kálmán, Czugler & Argay, 1981) of compounds containing (aryl)SO_2NX,X' (X,X' = H,C,N,S,P) groupings, show that for most of these compounds the torsion angles about the S—C(ring) bond fall in the range $|\varepsilon_1| = 70–120°$ and those about the S—N bond in the range $|\varepsilon_2| = 60–90°$. In the present structure the torsion angles C(5)—C(4)—S—N(2) = 85·6 (5), C(3)—C(4)—S—N(2) = −95·9 (5) and C(4)—S—N(2)—C(7) = 71·7 (5)°. The corresponding torsion angles in sulfisomidine base are 75·9, −104·4 and 59·1°, respectively, and they all lie within the range proposed by Kálmán *et al.* (1981). There is also a great deal of similarity in the other torsion angles about the S—C(ring) and S—N bonds in the two molecules, although they have crystallized in different environments (see Table 2). The dihedral angle between the phenyl and pyrimidine rings is 78·6 (5)°.

Table 2. *Bond lengths* (Å), *bond angles* (°) (*with e.s.d.'s in parentheses*) *and selected torsion angles* (°); *corresponding values for sulfisomidine base* (*Singh, Tiwari & Singh,* 1985) *are given for comparison*

	Sulfiso-midine. $2HCl.2H_2O$	Sulfiso-midine base		Sulfiso-midine. $2HCl.2H_2O$	Sulfiso-midine base
C(1)–C(2)	1·374 (4)	1·389 (6)	S–N(2)	1·654 (3)	1·630 (3)
C(2)–C(3)	1·366 (5)	1·382 (5)	N(2)–C(7)	1·373 (4)	1·342 (3)
C(3)–C(4)	1·384 (5)	1·390 (5)	N(3)–C(7)	1·347 (4)	1·363 (4)
C(4)–C(5)	1·387 (4)	1·377 (5)	N(3)–C(10)	1·318 (4)	1·323 (4)
C(5)–C(6)	1·360 (5)	1·374 (6)	N(4)–C(9)	1·363 (4)	1·355 (4)
C(1)–C(6)	1·376 (5)	1·383 (7)	N(4)–C(10)	1·343 (4)	1·335 (4)
N(1)–C(1)	1·464 (4)	1·370 (5)	C(8)–C(9)	1·358 (5)	1·349 (4)
S–C(4)	1·755 (3)	1·755 (3)	C(7)–C(8)	1·390 (5)	1·414 (4)
S–O(1)	1·435 (2)	1·430 (3)	C(9)–C(12)	1·485 (5)	1·487 (5)
S–O(2)	1·420 (2)	1·451 (2)	C(10)–C(11)	1·492 (5)	1·492 (5)

	Sulfisomidine. $2HCl.2H_2O$	Sulfisomidine base
O(1)–S–O(2)	120·5 (2)	115·9 (2)
O(1)–S–N(2)	109·8 (2)	112·3 (2)
O(1)–S–C(4)	108·3 (1)	108·7 (2)
O(2)–S–N(2)	102·9 (2)	103·8 (1)
O(2)–S–C(4)	109·0 (1)	106·4 (1)
N(2)–S–C(4)	105·3 (1)	109·5 (1)
C(1)–C(2)–C(3)	119·5 (3)	120·7 (4)
C(2)–C(3)–C(4)	120·1 (3)	120·0 (3)
C(3)–C(4)–C(5)	119·7 (3)	119·5 (3)
C(4)–C(5)–C(6)	120·0 (3)	120·0 (4)
C(1)–C(6)–C(5)	119·7 (3)	121·6 (4)
C(2)–C(1)–C(6)	121·0 (3)	118·1 (4)
N(1)–C(1)–C(2)	119·8 (3)	121·2 (4)
N(1)–C(1)–C(6)	119·1 (3)	120·7 (4)
S–C(4)–C(5)	120·4 (3)	119·7 (2)
S–C(4)–C(3)	119·8 (3)	120·9 (3)
S–N(2)–C(7)	127·8 (2)	120·4 (2)
N(2)–C(7)–N(3)	118·0 (3)	121·9 (3)
N(2)–C(7)–C(8)	118·8 (3)	118·1 (3)
C(7)–C(8)–C(9)	118·5 (3)	119·3 (3)
N(4)–C(9)–C(8)	117·1 (3)	119·7 (3)
C(9)–N(4)–C(10)	122·2 (3)	118·3 (3)
N(3)–C(10)–N(4)	122·3 (3)	122·1 (3)
C(7)–N(3)–C(10)	116·6 (3)	118·3 (3)
N(3)–C(7)–C(8)	123·2 (3)	120·0 (2)
C(8)–C(9)–C(12)	124·9 (3)	122·0 (2)
N(4)–C(9)–C(12)	118·0 (3)	116·3 (3)
N(3)–C(10)–C(11)	119·7 (3)	122·1 (3)
N(4)–C(10)–C(11)	118·0 (3)	118·3 (3)
C(3)–C(4)–S–O(2)	154·3*	144·0
C(3)–C(4)–S–O(1)	21·5	18·6
C(5)–C(4)–S–O(2)	−24·2	−35·7
C(5)–C(4)–S–O(1)	−157·0	−161·1
O(1)–S–N(2)–C(7)	−44·7	−61·7
O(2)–S–N(2)–C(7)	−174·2	172·4
S–N(2)–C(7)–C(8)	−171·9	180·0
S–N(2)–C(7)–N(3)	7·3	−1·21

* E.s.d.'s *ca* 0·5°.

The molecular packing of the title structure is shown in Fig. 2. The hydrogen-bond parameters have been deposited.* The crystal structure is stabilized by an intricate network of hydrogen bonds of types N—H···Cl, O—H···N and O—H···Cl. Both N(1) and N(4) are protonated, and all four H atoms attached to them participate in hydrogen bonding. The hydrogen bond involving one of the water molecules, O(*W*2), is rather weak. There is a short intermolecular contact distance between N(3) and O(1) [N(3)···O($1^{x,y,z+1}$) = 3·010 (3) Å].

We thank Professor E. F. Meyer Jr (for permitting the use of his Vector General Graphics System, Fig. 2) and Dr. Rosemarie Swanson of Texas A & M University, College Station, USA, for their help. We also thank Bhabha Atomic Research Centre for providing access to their IRIS 80 computer in Calcutta.

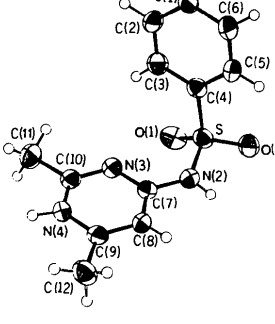

Fig. 1. Drawing of sulfisomidine dihydrochloride dihydrate with anisotropic thermal parameters at the 50% probability level. H atoms are shown as spheres of arbitrary radius. Protonation has occurred at N(1) and N(4).

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* See deposition footnote.

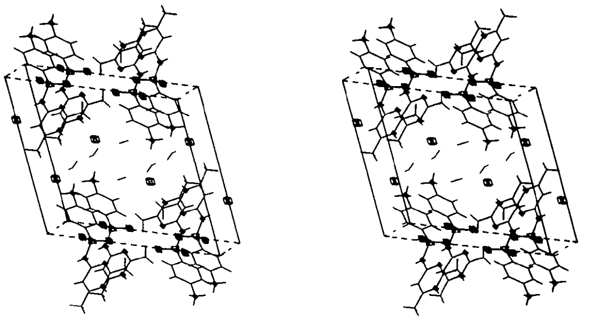

Fig. 2. Stereoview of the packing in the unit cell, viewed approximately along **c**. Unit-cell edges are indicated by a solid line for **a**, and dashed lines for **b**. N atoms are designated by tetrahedral symbols, O atoms by octahedra and Cl atoms by cubes. Drawing made by program *PACK* (Swanson, Rosenfield & Meyer, 1982).

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583 Pigment Yellow GG, A Mixed Crystal of α-(4-Chloro-2-nitrophenylhydrazono)acetoacetanilide (CI Pigment Yellow 6) and α-(2-Nitrophenylhydrazono)acetoacetanilide (α-CI Pigment Yellow 5)

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Abstract. Monoclinic, $P2_1/n$, $a = 7\cdot572\,(4)$, $b = 20\cdot366\,(4)$, $c = 10\cdot413\,(3)$ Å, $\beta = 98\cdot89\,(3)°$, $V = 1586\cdot5\,(0\cdot9)$ Å^3, $Z = 4$, $D_m = 1\cdot447\,(5)$ Mg m^{-3}. Assuming $C_{16}H_{13}ClN_4O_4$ ($M_r = 360\cdot76$), $D_x = 1\cdot510\,(1)$ Mg m^{-3}, $F(000) = 744$, $\lambda(\text{Mo } K\alpha) = 0\cdot71069$ Å, $\mu = 0\cdot22$ mm^{-1}. $R = 6\cdot5\%$ for 3123 non-zero intensities (room temperature). The structure was found to be a mixture of CI Pigment Yellow 6 ($C_{16}H_{13}ClN_4O_4$) ($0\cdot605 \pm 0\cdot003$) and α-CI Pigment Yellow 5 ($C_{16}H_{14}N_4O_4$). The molecule exists as the hydrazone tautomer and three intramolecular hydrogen bonds keep it approximately planar. The molecules are linked by van der Waals forces. The present structure is compared with four other pigment structures and it is concluded that it is a mixed crystal of CI Pigment Yellow 6 in α-CI Pigment Yellow 5 rather than *vice versa*.

Introduction. Pigments colour in the form of discrete crystalline particles. In view of this the colour properties depend not only upon the absorption properties of the molecule but also upon their crystallographic arrangement. This article is one of a group (Whitaker, 1983*a*,*b*, 1984*a*,*b*, 1985*a*,*b*; Whitaker & Walker, 1985) concerned with the structure of acetoacetanilide azo-pigments with the long-term aim of relating colour and crystal structure in pigments.

583 Pigment Yellow GG (commercially manufactured by Horace Cory & Co.) is nominally CI Pigment Yellow 6, $C_{16}H_{13}ClN_4O_4$, (CI 11670); the

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