with its reduced value possibly due to geminal non-bonded interactions of C10 and C14 with the large Te atom to which C9 is attached or to VSEPR effects. Steric effects, whether attributed to non-bonded atom interactions or to electron-pair repulsions, seem to be indicated by the angles C1—C2—C3 = 130·4 (5)° and Te—C1—C2 = 130·9 (4)°. A valuable scheme for the correlation of 1···3 intramolecular distances has been developed by Bartell and his co-workers (Bartell, 1968) and applied to a wide range of inorganic materials (*e.g.* O'Keeffe & Hyde, 1981). The distance C1···C3 = 2·513 Å is in good agreement with the value 2·50 Å predicted from the 1···3 radius for C of 1·25 Å. Since Te···C2 = 3·117 Å, the 1···3 radius for Te may be estimated to be 1·87 Å, compared to the van der Waals radius of 2·20 Å (Pauling, 1960). An earlier application of Bartell's idea to α-TeO_2 gave 1·87 Å for the estimated 1···3 radius for Te (Glidewell, 1979). There is a short Te···Te′ intermolecular contact of 3·84 Å, across the center at $\frac{1}{2},\frac{1}{2},\frac{1}{2}$, but the angles C1—Te—Te′ = 136° and C9—Te—Te′ = 77° do not have any obvious pictorial interpretation. All other intermolecular contact distances are normal.

The atoms C9, Te, C1, C2 and C3 lie close to one plane, with the phenyl ring C3–C8 rotated 10° from it in one direction and the other ring (C9–C14) turned 58° in the opposite sense. The planes O, C12, C15 and C9–C14 are rotated 1·7° from each other.

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References

Bartell, L. S. (1968). *J. Chem. Educ.* **45**, 754–767.

Cromer, D. T. & Liberman, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.

Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* A**24**, 321–324.

Dabdoub, M. J., Dabdoub, V. B., Comasseto, J. V. & Petragnani, N. (1986). *J. Organomet. Chem.* **308**, 211–222.

Domenicano, A., Murray-Rust, P. & Vaciago, A. (1983). *Acta Cryst.* B**39**, 457–468.

Domenicano, A., Vaciago, A. & Coulson, C. A. (1975). *Acta Cryst.* B**31**, 1630–1641.

Glidewell, C. (1979). *Inorg. Chim. Acta*, **12**, 219–227.

Husebye, S., Meyers, E. A., Zingaro, R. A., Braga, A. L., Comasseto, J. V. & Petragnani, N. (1986). *Acta Cryst.* C**42**, 1789–1792.

Lide, D. L. Jr (1962). *Tetrahedron*, **17**, 125–134.

O'Keeffe, M. & Hyde, B. G. (1981). *Structure and Bonding in Crystals*, Vol. I, edited by M. O'Keeffe & A. Navrotsky, pp. 227–254. New York: Academic Press.

Pauling, L. (1960). *The Nature of the Chemical Bond*, 3rd ed. Ithaca: Cornell Univ. Press.

Sheldrick, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.

Sheldrick, G. M. (1987). *SHELXTL-Plus*. Nicolet XRD Corporation, Madison, Wisconsin, USA.

Stewart, R. F., Davidson, E. R. & Simpson, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

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Structure of the 4-Phenyl-1,2-dithia-3,5-diazolium Chloride Adduct with Toluene, $C_7H_5N_2S_2^+.Cl^-.\frac{1}{6}C_7H_8$

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Abstract. M_r = 232·07, triclinic, $P\bar{1}$, a = 15·774 (10), b = 7·564 (5), c = 13·787 (9) Å, α = 100·23 (3), β = 109·85 (4), γ = 95·20 (4)°, V = 1502 (2) Å^3, Z = 6, D_x = 1·539 (2) Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 0·734 (1) mm^{-1}, $F(000)$ = 710, room temperature, $R(F)$ = 0·055 for 1523 reflexions [$I > 3\sigma(I)$] and 172 variables. There are three independent phenyldithiadiazolium ions in the asymmetric unit. The mean distances in the dithiadiazolium rings are S—S = 1·990 (3), S—N = 1·590 (4), C—N = 1·340 (5) Å. Each of the three independent cations has a Cl$^-$ close to its plane and about 2·9 Å from each S. There are also weak S—Cl interactions linking the disulfide groups and the chloride ions in planes parallel to (10$\bar{1}$). The toluene lies on a symmetry centre and is disordered.

Introduction. Short disulfide-to-anion distances have been observed in several compounds. In the cases where the disulfide group is part of an aromatic ring the anion is close to the plane of the ring and is approximately equidistant from the two S atoms (Andreasen, Hazell & Hazell, 1977, and references therein). The structure of 4-phenyl-1,2-dithia-3,5-diazolium chloride (Alange, Banister, Bell & Millen, 1977) has been determined for comparison with related compounds.

Experimental. The compound, which was provided by Dr A. J. Banister, recrystallized from toluene as orange-yellow needles. A crystal of dimensions 0·10 × 0·06 × 0·75 mm was mounted on a Picker FACS-1 diffractometer and cell dimensions determined from the

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Table 1. *Coordinates in an orthogonal system* (Å) *with* $X \parallel a$, $Z \parallel c^*$ *and* Y *perpendicular to* X *and* Z *and origins* (O) *of the axial systems* (Å) *for the toluenes*

	X	Y	Z
Cl(1)	6·058 (3)	0·420 (3)	5·384 (3)
Cl(2)	9·196 (3)	−3·436 (4)	8·658 (4)
Cl(3)	3·570 (3)	4·432 (4)	2·971 (4)
S(1)	4·186 (3)	1·056 (4)	7·523 (4)
N(1)	2·939 (9)	1·145 (10)	8·512 (9)
S(2)	3·520 (4)	−0·516 (4)	6·499 (3)
N(2)	2·166 (10)	−0·685 (10)	7·314 (9)
S(3)	6·776 (3)	−4·326 (3)	10·006 (4)
N(3)	5·647 (9)	−4·582 (9)	11·089 (9)
S(4)	7·574 (3)	−2·764 (4)	10·943 (4)
N(4)	6·586 (9)	−2·789 (10)	12·195 (9)
S(5)	1·961 (3)	3·494 (4)	5·240 (4)
N(5)	0·804 (9)	3·260 (10)	6·293 (10)
S(6)	0·945 (3)	4·766 (4)	4·093 (4)
N(6)	−0·402 (9)	4·684 (10)	4·944 (10)
O(1)	1·977 (8)	0·234 (9)	8·288 (8)
O(2)	5·667 (7)	−3·726 (8)	12·143 (8)
O(3)	−0·343 (8)	3·931 (9)	6·026 (8)
O(4)	−0·813 (45)	1·175 (76)	0·655 (46)

Table 2. *Coordinates* (Å) *of the toluene fragments relative to the inertial axes*

	X	Y	Z
C(1)	0·000	0·000	0·000
C(2)	−1·479 (8)	0·000	0·000
C(3)	−2·172 (7)	1·201 (5)	0·000
C(4)	−3·542 (8)	1·195 (6)	0·000
C(5)	−4·227 (8)	0·000	0·000
C(6)	−2·172 (7)	−1·201 (5)	0·000
C(7)	−3·542 (8)	−1·195 (6)	0·000

Table 3. *Euler angles* (°), *as defined in Goldstein* (1969)

	φ	θ	ψ
Cation 1	227·2 (3)	56·5 (2)	−214·7 (3)
Cation 2	−54·8 (2)	121·2 (2)	−42·0 (3)
Cation 3	221·2 (2)	117·8 (3)	−165·4 (3)
Toluene	159·8 (1·6)	39·6 (6)	−61·9 (1·4)

Table 4. *Thermal parameters* **T** (Å²), **L** *and extra oscillation parameter* (°²), 10**S** (° Å) *and the centres of libration* (Å) *for the three cations* (1–3) *and the toluene* (*tol.*)

ij	11	22	33	23	31	12	Osc.
T1	1·14 (4)	0·88 (7)	0·88 (6)	0·15 (5)	−0·17 (4)	0·11 (4)	
T2	0·84 (6)	0·87 (7)	0·82 (6)	0·19 (5)	−0·04 (4)	0·12 (5)	
T3	0·96 (4)	0·91 (9)	1·13 (7)	−0·11 (5)	0·05 (4)	−0·05 (4)	
Ttol.	2·37 (66)	7·67 (1·03)	1·79 (35)	−3·47 (45)	0·29 (36)	0·68 (61)	
L1	0·39 (6)	0·06 (1)	0·20 (4)	−0·00 (1)	−0·23 (4)	0·00 (2)	−0·21 (25)
L2	0·18 (4)	0·06 (1)	0·28 (4)	−0·03 (2)	−0·20 (3)	0·02 (2)	−0·01 (25)
L3	0·37 (6)	0·06 (1)	0·20 (4)	−0·01 (1)	−0·24 (4)	0·02 (4)	0·14 (30)
Ltol.	0·26 (16)	0·25 (20)	1·08 (27)	−0·71 (21)	0·01 (16)	0·18 (16)	

ij	23	31	12	32	13	21	33—22	11—33
S1	1 (7)	2 (13)	3 (20)	3 (15)	34 (17)	−14 (7)	−46 (14)	−19 (24)
S2	−5 (7)	8 (26)	7 (27)	−4 (27)	−34 (21)	18 (8)	−9 (22)	−26 (44)
S3	6 (6)	2 (12)	14 (31)	−3 (25)	16 (21)	10 (6)	−19 (20)	−4 (27)

	X	Y	Z
1	2·250	0·261	8·247
2	4·562	−4·057	13·265
3	−0·819	3·880	6·204
Tol.	−0·904 (327)	4·245 (609)	−1·312 (1·379)

setting angles of 15 reflexions with $19 < 2\theta < 27°$. Intensities were measured out to $2\theta_{\max} = 38°$ with graphite-monochromated Mo $K\alpha$ radiation using an ω–2θ scan. The 2θ-scan width was $(3{\cdot}92 + 0{\cdot}692\tan\theta)°$ for k positive and $(3{\cdot}0 + 0{\cdot}692\tan\theta)°$ for k negative. The step length was 0·04°, the counting time 2 s step^{-1}. Reflexions with $-14 \le h \le 14$, $-6 \le k \le 6$, $-12 \le l \le 12$ were measured giving 2414 independent reflexions, $R_{\text{int}} = 0{\cdot}053$, of which 1523 had $I > 3\sigma(I)$. Reflexions $\bar{4}2\bar{4}$ and 120 were monitored every 30 reflexions, the overall fall off in intensity was 19%. No corrections were made for absorption.

MULTAN (Germain, Main & Woolfson, 1971) gave the positions of the three dithiadiazolium chloride ion pairs in the asymmetric unit. A Fourier synthesis showed the crystal to contain solvent molecules, the toluene being disordered and close to a symmetry centre. Least-squares refinement was carried out using the constrained-refinement technique (Pawley, 1971) to limit the number of variables. Chloride ions were not constrained and their thermal motion was described in terms of U_{ij}. Thermal motion of the cations was described by **T**, **L** and **S** and an additional parameter for the oscillation of the benzene ring about the aliphatic C—C bond relative to the dithiadiazole, and for the toluene by **T**, **L** and **X**. The C_6H_5C fragments of the cations and of the toluene were constrained to be identical and to have *mm*2 symmetry. The positions of the aromatic H atoms were calculated for each cycle assuming C—H = 0·95 Å and assuming the C—H bond to bisect the C—C—C angle. The positions of the S and the N atoms were not constrained. The weighting scheme was $w = 1/\sigma^2(F)$ where $\sigma(F) = [\sigma_{\text{CS}}(F^2) + 1{\cdot}03F^2]^{1/2} - |F|$ and $\sigma_{\text{CS}}(F^2)$ is the standard deviation of F^2 from counter statistics. Refinement (on F) gave $R = 0{\cdot}055$, $wR = 0{\cdot}079$, $S = 2{\cdot}74$ for 172 variables and 1522 reflexions $[I > 3\sigma(I)]$, $(\Delta/\sigma)_{\max} = 0{\cdot}7$, $\Delta\rho = 0{\cdot}30$ (3) to $-0{\cdot}41$ (8) e Å^{-3}. Coordinates for Cl, S, N and the origins of the axial systems for the toluene fragments are listed in Table 1, coordinates of C atoms in Table 2, Euler angles in Table 3, **T**, **L** and **S** in Table 4 and distances and angles in Table 5.*

Computations were carried out on a VAX 11/780 computer with the following programs: *PROCH*, *DATAP* and *DSORT* (State University of New York) – data processing; *KONSTR* – least-squares refinement; *ORTEP* (Johnson, 1965) – drawings. Scattering curves those of Cromer & Mann (1968) for Cl, S and C, those of Stewart, Davidson & Simpson (1965) for H.

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* Lists of structure factors, fractional coordinates and anisotropic thermal parameters and some angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51090 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 5. *Bond distances* (Å), S—Cl *distances* < 3·65 Å *and bond angles* (°)

Symmetry code: (i) 1−*x*, 1−*y*, 1−*z*; (ii) 1−*x*, −*y*, 1−*z*.

S(1)—S(2)	1·991 (5)	S(3)—S(4)	1·989 (5)	S(5)—S(6)	1·991 (5)
S(1)—N(1)	1·594 (10)	S(3)—N(3)	1·585 (10)	S(5)—N(5)	1·581 (10)
S(2)—N(2)	1·590 (10)	S(4)—N(4)	1·595 (10)	S(6)—N(6)	1·595 (10)
N(1)—C(1)	1·345 (13)	N(3)—C(8)	1·358 (12)	N(5)—C(15)	1·356 (13)
N(2)—C(1)	1·351 (13)	N(4)—C(8)	1·314 (12)	N(6)—C(15)	1·320 (13)
C(2)—C(3)	1·387 (10)	C(3)—C(4)	1·370 (9)	C(4)—C(5)	1·378 (11)
C(1)—C(2)	1·479 (8)				
Cl(1)—S(1)	2·912 (5)	Cl(2)—S(3)	2·910 (5)	Cl(3)—S(5)	2·936 (5)
Cl(1)—S(2)	2·925 (5)	Cl(2)—S(4)	2·881 (5)	Cl(3)—S(6)	2·874 (5)
Cl(1)—S(1^{i})	3·187 (5)	Cl(2)—S(2^{ii})	3·177 (5)	Cl(3)—S(3^{ii})	3·101 (5)
Cl(1)—S(5^{i})	3·211 (5)	Cl(2)—S(5^{ii})	3·201 (5)	Cl(3)—S(4^{i})	3·322 (5)
Cl(1)—S(2^{ii})	3·263 (5)	Cl(2)—S(6^{i})	3·331 (5)	Cl(3)—S(1^{i})	3·515 (5)
Cl(1)—S(3^{ii})	3·409 (5)				

S(1)—Cl(1)—S(2)	39·9 (1)	S(3)—Cl(2)—S(4)	40·2 (1)	S(5)—Cl(3)—S(6)	40·1 (1)
Cl(1)—S(1)—S(2)	70·4 (1)	Cl(2)—S(3)—S(4)	69·2 (1)	Cl(3)—S(5)—S(6)	68·3 (1)
Cl(1)—S(2)—S(1)	69·7 (1)	Cl(2)—S(4)—S(3)	70·7 (1)	Cl(3)—S(6)—S(5)	71·6 (2)
Cl(1)—S(1)—N(1)	166·0 (2)	Cl(2)—S(3)—N(3)	163·4 (2)	Cl(3)—S(5)—N(5)	164·3 (2)
Cl(1)—S(2)—N(2)	165·5 (2)	Cl(2)—S(4)—N(4)	165·3 (2)	Cl(3)—S(6)—N(6)	166·8 (3)
S(1)—S(2)—N(2)	96·0 (3)	S(3)—S(4)—N(4)	96·3 (3)	S(5)—S(6)—N(6)	95·2 (3)
S(2)—S(1)—N(1)	95·8 (3)	S(4)—S(3)—N(3)	95·2 (3)	S(6)—S(5)—N(5)	96·0 (3)
S(1)—N(1)—C(1)	114·8 (7)	S(3)—N(3)—C(8)	114·7 (6)	S(5)—N(5)—C(15)	114·5 (7)
S(2)—N(2)—C(1)	114·6 (7)	S(4)—N(4)—C(8)	114·4 (7)	S(6)—N(6)—C(15)	115·4 (7)
N(1)—C(1)—N(2)	118·7 (8)	N(3)—C(8)—N(4)	119·4 (7)	N(5)—C(15)—N(6)	118·8 (8)
C(2)—C(1)—N(1)	119·9 (8)	C(9)—C(8)—N(3)	119·2 (8)	C(16)—C(15)—N(5)	120·9 (8)
C(2)—C(1)—N(2)	121·0 (8)	C(9)—C(8)—N(4)	121·4 (8)	C(16)—C(15)—N(6)	120·2 (8)
C(3)—C(2)—C(6)	120·0 (7)	C(1)—C(2)—C(3)	120·0 (6)	C(2)—C(3)—C(4)	119·8 (6)
C(3)—C(4)—C(5)	120·1 (6)	C(4)—C(5)—C(7)	120·3 (7)		

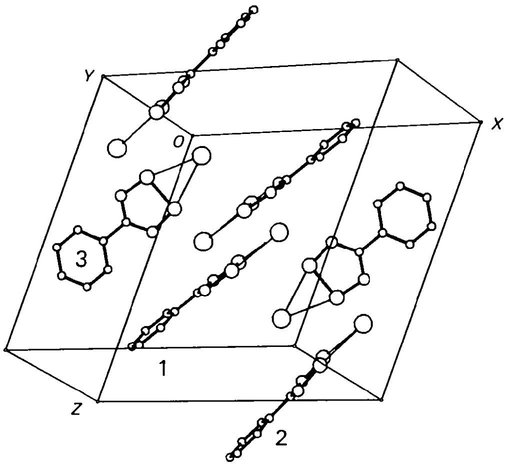

Fig. 1. The unit-cell contents showing the three independent dithiadiazolium chlorides. The radii of the circles increase with the atomic number of the atoms they represent.

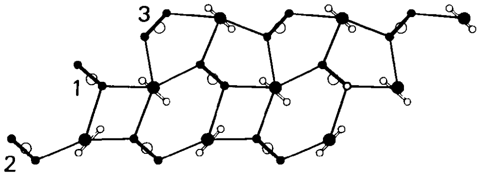

Fig. 2. Two layers of S and Cl atoms showing the interactions within one of the layers, thick lines represent S—S bonds. **b** is across the page, [10$\bar{1}$] makes an angle of 10° with the page. The atoms represented by filled circles are *ca* 2·7 Å above those shown as open circles.

Discussion. There are three independent phenyldithiadiazolium ions in the asymmetric unit (Fig. 1). In each case the benzene ring and a chloride ion are approximately coplanar with the dithiadiazolium group. The chloride ions are roughly equidistant from the two S atoms, S—Cl distances ranging from 2·874 (5) to 2·936 (5) Å with a mean of 2·906 (2) Å. This distance is intermediate between that of 2·0 Å for an S—Cl covalent bond and the value 3·6 Å calculated from Pauling's (1960) radii assuming a charge of $+\frac{1}{2}$ on each S. The S—Cl distances are similar to those of 2·837 (6) and 2·874 (6) Å in $\mathrm{CCl_3CN_2S_2^+.Cl^-}$ (Andreasen *et al.*, 1977) and 2·801 (2) to 2·926 (2) Å in $\mathrm{S_4N_3^+.Cl^-}$ (Svenningsen & Hazell, unpublished). There are also weak interactions with S···Cl ranging from 3·1 to 3·5 Å (*cf.* the sum of the van der Waals radii 3·65 Å). The disulfide groups and the chloride ions of symmetry-related ion pairs lie on two layers, 2·7 Å apart, parallel to (10$\bar{1}$). The weak interactions all lie in these layers (Fig. 2), the two layers being linked by the short S—Cl bonds. There are no short S···S or Cl···Cl distances. The S—Cl bonds are not quite equal and the alternation extends round the dithiadiazole ring. Ion pair 1 has the most symmetric environment, two weak interactions to each S and four to Cl⁻, and is itself the most symmetric. Ion pairs 2 and 3 have less symmetric arrangements, two weak interactions to one S and one to the other and three interactions to the Cl⁻. The Cl⁻ ions are displaced towards the missing fourth interaction giving short S(4)—Cl and S(6)—Cl distances, S(4) and S(6) being the S atoms with only one weak S···Cl interaction. The S—S bond length of 1·990 (3) Å

Table 6. *Geometry* (Å) *of* 1,2-*dithia*-3,5-*diazoles*

	S—S	S—N	N—C	Reference
Ion				
$PhCN_2S_2^+$	1·990 (3)	1·590 (4)	1·340 (5)	*a*
$CCl_3CN_2S_2^+$	2·009 (6)	1·583 (7)	1·318 (10)	*b*
$ClCN_2S_2^+$	1·996 (2)	1·573 (3)	1·321 (6)	*c*
$CF_3CN_2S_2^+$	1·989 (3)	1·589 (4)	1·323 (7)	*d*
Dimer				
$[PhCN_2S_2]_2$	2·089	1·625	1·338	*e*
$[CF_3CN_2S_2]_2$	2·087 (1)	1·630 (2)	1·318 (2)	*d*
$[CF_3CN_2S_2]_2$	2·086 (1)	1·640 (2)	1·328 (4)	*d*
Monomer				
$CF_3CN_2S_2$(gas)	2·113 (6)	1·623 (3)	1·318 (6)	*d*

References: (*a*) This work; (*b*) Andreasen *et al.* (1977); (*c*) Höfs, Mews, Clegg, Noltemeyer, Schmidt & Sheldrick (1983); (*d*) Höfs *et al.* (1985); (*e*) Vegas *et al.* (1980).

is significantly shorter than that, 2·089 Å, in the corresponding phenyldithiadiazole dimer (Vegas, Pérez-Salazar, Banister & Hey, 1980), which is in agreement with the trend, Table 6, for the dimer to have an S—S bond intermediate between that of the 6π dithiadiazolium ion and the 7π dithiadiazole radical. The S—N bond of 1·590 (4) Å is also shorter than that of the dimer. There is a wide variation in the C—N distances, the longest being those of the phenyl derivatives.

References

ALANGE, G. G., BANISTER, A. J., BELL, N. & MILLEN, P. W. (1977). *Inorg. Nucl. Chem. Lett.* **13**, 143–144.

ANDREASEN, O., HAZELL, A. C. & HAZELL, R. G. (1977). *Acta Cryst.* B**33**, 1109–1112.

CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* A**24**, 321–324.

GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* A**27**, 368–376.

GOLDSTEIN, H. (1969). *Classical Mechanics*, p. 107. Reading, MA: Addison–Wesley.

HÖFS, H.-U., BATS, J. W., GLEITER, R., HARTMANN, G., MEWS, R., ECKERT-MAKSIĆ, M., OBERHAMMER, H. & SHELDRICK, G. M. (1985). *Chem. Ber.* **118**, 3781–3804.

HÖFS, H.-U., MEWS, R., CLEGG, W., NOLTEMEYER, M., SCHMIDT, M. & SHELDRICK, G. M. (1983). *Chem. Ber.* **116**, 416–423.

JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

PAULING, L. (1960). *The Nature of the Chemical Bond*, 3rd ed., pp. 511–518. Ithaca: Cornell Univ. Press.

PAWLEY, G. S. (1971). *Adv. Struct. Res. Diffr. Methods*, **4**, 1–64.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

VEGAS, A., PÉREZ-SALAZAR, A., BANISTER, A. J. & HEY, R. G. (1980). *J. Chem. Soc. Dalton Trans.* pp. 1812–1815.

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Structural Studies on Molecular Complexes. II. Structure of Aminacrine–Sulfadimidine (1/1)

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Abstract. 1:1 molecular complex of 9-aminoacridine and N^1-(4,6-dimethyl-2-pyrimidinyl)sulfanilamide, $C_{13}H_{11}N_2^+.C_{12}H_{13}N_4O_2S^-$, $M_r = 472·57$, monoclinic, $P2_1/c$, $a = 12·131$ (1), $b = 12·266$ (1), $c = 16·287$ (2) Å, $\beta = 103·79$ (1)°, $V = 2353·6$ Å^3, $Z = 4$, $D_m = 1·34$, $D_x = 1·33$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda(\alpha_1) = 0·7093$ Å, $\mu = 1·64$ cm^{-1}, $F(000) = 992$, $T = 295$ K, $R = 0·036$ for 1847 reflections. The structure contains an acridinium–sulfanilamidate ion pair with a strong N(acridinium)—H···N(pyrimidinyl) hydrogen bond. Some structural changes of the individual species in the molecular complex are discussed.

Introduction. Sulfonamides have been reported to form association complexes with a variety of small molecules (Shefter & Sackman, 1971). 9-Aminoacridine has been combined with sulfa drugs by salt linkages, and the resulting compounds were found to have synergistic antimicrobial activity (McIntosh, Robinson & Selbie, 1945; Dasgupta & Gupta, 1946), and some of them were used clinically for a long time. We have carried out X-ray crystallographic studies of a few such

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