$C_{19}H_{23}ClN_4O_3S$ AND $C_{20}H_{25}ClN_4O_3S$

Fig. 2. A stereoview of the contents of one unit cell for ACLSA.

torsion angles C(6)—C(1)—N(1)—N(2) and C(2)—C(1)—N(1)—N(2) are −4·2 (4) and 176·0 (3)° in ACLSA and 8·0 (6) and −172·0 (5)° in CLSPA.

In both structures the molecular packing involves normal van der Waals contacts, with no intermolecular hydrogen bonding. A stereoview of the contents of one unit cell (Johnson, 1965) is shown for ACLSA in Fig. 2.

The results of the crystal structure analyses of these two dyes do not reveal any marked changes in molecular geometry which could be the cause of their different fiber affinity, nor have any such changes been observed between ABRCA (Handal, Gruska & White, 1980) and BRCPA (Handal & White, 1980). The differing affinities may be due to a critical molecular

volume (Gerber, 1976) or to an important change in physical properties caused by the subtle chemical change.

We thank Dr E. J. Moriconi and Sandoz Ltd for crystals of the title compounds.

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[(1RS,2RS,3SR)-3-Hydroxy-2-methylcyclopentyl]trimethylammonium Chloride

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Abstract. $C_9H_{20}NO^+.Cl^-$, $M_r = 193.72$, orthorhombic, $P2_12_12_1$, $a = 7.440$ (2), $b = 11.609$ (2), $c = 12.295$ (3) Å, $U = 1061.9$ Å, $Z = 4$, $D_x = 1.212$ Mg m^{-3}, μ(Mo Kα) = 0·32 mm^{-1}. The structure was refined to $R = 0.0415$ for 985 independent reflexions. The five-membered ring adopts the envelope conformation; the three substituents are cis. The two ions are linked by an O—H···Cl hydrogen bond.

Introduction. The structure of the title compound has been determined to elucidate the arrangement of substituents on the five-membered ring. As frequently found for saturated C_5 rings, rapid conformational changes in solution (pseudorotation) ruled out an unambiguous structural assignment on the basis of NMR data alone.

Hygroscopic crystals were obtained from ethanol/diethyl ether and sealed in Lindemann capillaries. Data were collected on a Stoe–Siemens four-circle diffractometer with a control program written by Clegg (1981) and a crystal 0·3 × 0·3 × 0·4 mm. 1093 data were recorded for $7 < 2\theta < 50°$; after averaging

Table 1. *Atom coordinates* $(\times 10^4)$ *and isotropic temperature factors* $(\text{Å}^2 \times 10^3)$

	x	y	z	U
H(10)	1981 (66)	−1687 (45)	−1336 (40)	141 (11)
O	1794 (3)	−1586 (2)	−771 (2)	55 (1)*
N	7019 (3)	446 (2)	959 (2)	37 (1)*
C(1)	5641 (4)	−507 (2)	741 (2)	35 (1)*
H(1)	6477	−1135	700	44
C(2)	4584 (4)	−486 (2)	−331 (2)	37 (1)*
H(2)	5343	−516	−961	44
C(3)	3335 (4)	−1516 (3)	−88 (2)	47 (1)*
H(3)	3973	−2221	−220	61
C(4)	2755 (5)	−1347 (4)	1082 (3)	63 (1)*
H(4)	1655	−915	1110	81
H(4')	2584	−2079	1430	81
C(5)	4264 (4)	−676 (3)	1638 (2)	46 (1)*
H(5)	4764	−1113	2228	58
H(5')	3838	51	1906	58
C(6)	3550 (5)	588 (3)	−607 (2)	54 (1)*
H(6)	4333	1160	−913	68
H(6')	2989	890	35	68
H(6'')	2644	387	−1129	68
C(7)	8379 (4)	485 (3)	59 (2)	52 (1)*
H(7)	8912	−264	−14	64
H(7')	9297	1039	226	64
H(7'')	7802	694	−611	64
C(8)	7986 (5)	149 (3)	1993 (2)	62 (1)*
H(8)	8992	658	2081	76
H(8')	8403	−633	1979	76
H(8'')	7169	249	2590	76
C(9)	6262 (5)	1640 (3)	1069 (3)	55 (1)*
H(9)	5215	1622	1525	71
H(9')	5943	1936	366	71
H(9'')	7156	2128	1392	71
Cl	1624 (1)	2246 (1)	1983 (1)	52 (1)*

* $U = \frac{1}{3}$ of the trace of the orthogonalized U_{ij} matrix.

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

C(1)−N	1·532 (5)		C(1)−C(2)	1·535 (5)
C(1)−C(5)	1·517 (5)		C(2)−C(3)	1·544 (5)
C(2)−C(6)	1·504 (5)		C(3)−O	1·423 (5)
C(3)−C(4)	1·515 (5)		C(4)−C(5)	1·528 (6)
C(7)−N	1·501 (5)		C(8)−N	1·501 (5)
C(9)−N	1·502 (5)			
C(1)−N−C(7)	110·1 (3)		C(1)−N−C(8)	107·6 (3)
C(7)−N−C(8)	108·0 (3)		C(1)−N−C(9)	115·6 (3)
C(7)−N−C(9)	106·9 (3)		C(8)−N−C(9)	108·4 (3)
N−C(1)−C(2)	118·8 (3)		N−C(1)−C(5)	114·7 (3)
C(2)−C(1)−C(5)	106·3 (3)		C(1)−C(2)−C(3)	97·5 (3)
C(1)−C(2)−C(6)	118·0 (3)		C(3)−C(2)−C(6)	112·2 (4)
O−C(3)−C(2)	114·5 (3)		O−C(3)−C(4)	109·8 (4)
C(2)−C(3)−C(4)	104·7 (4)		C(3)−C(4)−C(5)	106·3 (4)
C(1)−C(5)−C(4)	103·7 (3)			

Table 3. *Torsional angles* (°)

The sign convention is as defined by Klyne & Prelog (1960).

C(7)−N−C(1)−C(2)	−56·5 (4)		C(6)−C(2)−C(3)−O	39·0 (4)		N−C(1)−C(2)−C(6)	−55·1 (4)
C(8)−N−C(1)−C(2)	−174·0 (3)		O−C(3)−C(4)−C(5)	−151·0 (4)		C(5)−C(1)−C(2)−C(6)	76·0 (4)
C(9)−N−C(1)−C(2)	64·7 (4)		C(3)−C(4)−C(5)−C(1)	−0·3 (4)		C(2)−C(1)−C(5)−C(4)	28·6 (4)
N−C(1)−C(2)−C(3)	−175·2 (3)		C(7)−N−C(1)−C(5)	176·3 (3)		C(1)−C(2)−C(3)−C(4)	43·1 (4)
C(5)−C(1)−C(2)−C(3)	−44·1 (4)		C(8)−N−C(1)−C(5)	58·8 (4)		C(6)−C(2)−C(3)−C(4)	−81·3 (4)
N−C(1)−C(5)−C(4)	161·9 (3)		C(9)−N−C(1)−C(5)	−62·5 (4)		C(2)−C(3)−C(4)−C(5)	−27·6 (4)
C(1)−C(2)−C(3)−O	163·4 (3)						

equivalents there remained 985 unique data with $F > 4\sigma(F)$, which were employed for the structure solution and refinement. The structure was solved by Patterson and Fourier methods and refined with complex neutral-atom scattering factors, anisotropic non-hydrogen atoms and weights $w = 1/[\sigma^2(F) + 0\cdot001F^2]$. The hydroxyl H atom was located in a difference synthesis and refined independently with an individual temperature factor. The remaining H atoms were given fixed isotropic temperature factors of 1·2 times the equivalent U of the C atom to which they were attached, and refined with riding constraints (CH, CH$_2$) or as rigid groups (CH$_3$) (C−H 0·96 Å, H−C−H 109·5°). Refinement converged to $R' = \sum w^{1/2} \Delta / \sum w^{1/2} |F_o| = 0\cdot0445$ with a corresponding R of 0·0415. Refinement of the enantiomeric structure gave almost identical R values. This lack of sensitivity to the absolute configuration may have been caused by microcrystalline twinning; the sample employed was racemic. Final atomic coordinates are given in Table 1,* bond lengths, angles and selected torsion angles in Tables 2 and 3. A view of the cation is given in Fig. 1.

Discussion. The five-membered ring has the all-*cis* configuration and adopts the envelope conformation with C(2) out of the plane of the other four ring atoms.
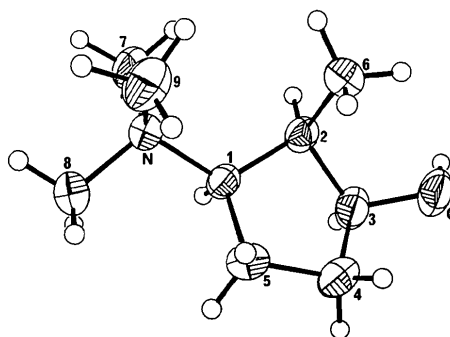
Fig. 1. The cation, with 50% probability thermal ellipsoids for the non-hydrogen atoms.

$C_9H_{20}NO^+ . Cl^-$

This conformation minimizes repulsion between the three substituents. The hydroxyl and $(CH_3)_3N$ groups are thus equatorial, the methyl substituent is axial. The maximum deviation from the cyclopentane torsion angles is $4°$. The crystal is constructed from ion pairs in which the ions are linked by an $O-H \cdots Cl$ hydrogen bond $|O \cdots Cl\ 3·096\ (6),\ H(10) \cdots Cl\ 2·33\ (2)\ Å|$.

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SHORT COMMUNICATIONS

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Lattice constants of the compounds Sr₂LnAlO₅ and Sr₂LnFeO₅.

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Abstract

Lattice parameters of the compounds $Sr_2Ln(Al,Fe)O_5$ were determined and the non-linearity of the r vs $V^{1/3}$ plot is discussed.

As part of the research program on the structural and magnetic properties of the compositions in the ternary system $SrO-Ln_2O_3-Fe_2O_3$, crystals of compounds with the general formula $Sr_2Ln(Al,Fe)O_5$ were prepared and the lattice parameters were redetermined. The crystals used for the lattice determination were prepared by the HST method (Drofenik, Golič & Kolar, 1979).

The cell parameters given in Table 1 were measured at $293·2\ (5)$ K using an Enraf–Nonius CAD-4 diffractometer.

They were determined by least-squares refinement of 45 reflection angles in the range $10 < \theta < 25°$, centered at $\pm 2\theta$ using graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0·70930$ Å).

In Fig. 1 the plot of ionic radius, r, vs $V^{1/3}$ is presented, where V is the cell volume of the structure. Values of $^{VIII}r^*$ were taken from the Shannon (1976) ionic radii. Good agreement was found for all rare-earth ions except La^{3+}. Since the detailed structure of Sr_2LaAlO_5 was not known, one would suppose that the coordination number of La^{3+} is not similar to that of the other rare-earth ions in this isostructural series, namely eight (Drofenik & Golič, 1979).

* The convention of Shannon (1976) is followed in this paper whereby a coordination number is denoted by a preceding Roman superscript. Thus ^{VIII}r is the effective radius of the particular species when eightfold coordinated.
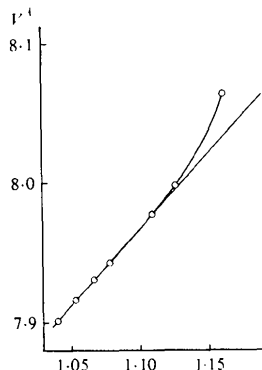
Table 1. *Comparison of cell parameters* (Å), *ionic radii* (Å) *and* $V^{1/3}$ (Å) *for some related compounds*

	a	c	^{VIII}r	$V^{1/3}$
Sr₂LaAlO₅	6·885 (1)	11·059 (1)	1·160	8·063
Sr₂PrAlO₅	6·809 (1)	11·032 (1)	1·126	7·997
Sr₂NdAlO₅	6·791 (1)	11·004 (1)	1·109	7·976
Sr₂SmAlO₅	6·757 (1)	10·972 (2)	1·079	7·942
Sr₂EuAlO₅*	6·742 (1)	10·970 (1)	1·066	7·930
Sr₂GdAlO₅	6·735 (1)	10·937 (2)	1·053	7·916
Sr₂TbAlO₅	6·717 (1)	10·932 (2)	1·040	7·901
Sr₂SmFeO₅	6·822 (1)	11·267 (2)		
Sr₂EuAlO₅*	6·812 (3)	11·263 (3)		
Sr₂GdFeO₅	6·805 (2)	11·263 (4)		

* Already published in Drofenik & Golič (1979).

Fig. 1. r (Å) vs $V^{1/3}$ (Å) for the first seven structures in Table 1.