Enraf–Nonius (1979). *Structure Determination Package*. Enraf–Nonius, Delft.

International Tables for X-ray Crystallography (1968). Tome III, p. 273, Tableau 4.2.5. Birmingham: Kynoch Press. (Distributeur actuel D. Reidel, Dordrecht.)

International Tables for X-ray Crystallography (1974). Tome IV, p. 72. Birmingham: Kynoch Press. (Distributeur actuel D. Reidel, Dordrecht.)

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

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1982). *MULTAN11/82. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. de York, Angleterre, et Louvain, Belgique.

WYCKOFF, R. W. G. (1969). *Crystal Structures*, Tome 6, 1ère partie, 2ème éd., p. 201. New York: Wiley–Interscience.

5-(2-Undecyloxyphenyl)-4,6-dithianonanedioic Acid

BY DRAKE S. EGGLESTON* AND CARL D. PERCHONOCK†

Smith Kline & French Laboratories, 1500 *Spring Garden Street, PO Box* 7929, *Philadelphia, PA* 19101, *USA*

Abstract. $C_{24}H_{38}O_5S_2$, $M_r = 470.70$, triclinic, $P\bar{1}$, $a = 12.988$ (4), $b = 19.213$ (5), $c = 5.507$ (1) Å, $\alpha = 94.80$ (2), $\beta = 97.95$ (2), $\gamma = 71.83$ (2)°, $V = 1291.8$ Å^3, $Z = 2$, D_m(flotation in aqueous $ZnCl_2$) $= 1.20$, $D_x = 1.210$ g cm^{-3}, $\lambda(Mo\, K\alpha_{1,2}) = 0.70926$, 0.71354 Å, $\mu = 2.26$ cm^{-1}, $F(000) = 508$, $T = 293$ K, $R = 0.041$, $wR = 0.051$ for 3400 observations. The 5-(2-undecyloxyphenyl)-4,6-dithianonanedioic acid molecule is a member of a novel class of selective leukotriene antagonists. Its molecular structure in the solid state shows a highly extended (all *trans*) undecane C chain. One of the two carboxylic acid arms of the dithioacetal moiety is extended nearly parallel to the undecane chain while the other projects nearly perpendicularly to the remainder of the molecule. Both mercaptopropionate chains are highly extended; however, the fully *trans* conformation of one contrasts to the *gauche–gauche–trans* conformation of the other. Individual molecules are related through strong hydrogen bonds between carboxylic acid groups 'dimerically' across crystallographic inversion centers.

Introduction. Leukotrienes C_4, D_4 and E_4 are now recognized as the integral components of slow reacting substance of anaphylaxis. Their release upon antigenic challenge of human and animal lung tissue (Lewis, Austen, Drazen, Clark, Marfat & Corey, 1980; Dahlen, Hansson, Hedquist, Bjorck, Granstrom & Dahlen, 1983) causes potent bronchoconstriction (Dahlen, Hedquist, Hammarstrom & Samuelson, 1980), increased microvascular permeability (Peck, Piper & Williams, 1981; Woodward, Weichman, Gill & Wasserman, 1983) and altered mucous production and transport (Marom, Shelhamer, Bach, Morton & Kaliner, 1982). Since these symptoms are associated with such ailments as allergic asthma it is believed that leukotriene antagonists will provide novel and effective therapy for such conditions.

Guided by the structures of the natural leukotrienes we are pursuing synthetic and structural studies aimed at discovering potent leukotriene antagonists. These efforts first led to the synthesis and pharmacological characterization of (4*R*,5*S*)-5-cysteinylglycyl-4-hydroxy-(*Z*)-6-nonadecenoic acid (1) (Gleason, Ku, McCarthy, Weichman, Holden, Osborn, Zabko-Potapovich, Berkowitz & Wasserman, 1983; Weichman, Wasserman, Holden, Osborn, Woodward, Ku & Gleason, 1983) and its analogs (Perchonock, Uzinskas, Ku, McCarthy, Bondinell, Volpe, Gleason, Weichman, Muccitelli, DeVan, Tucker, Vickery & Wasserman, 1985; Ku, McCarthy, Weichman & Gleason, 1985) as modestly potent antagonists. Some of these molecules, however, also display partial agonist properties. Further research has now identified certain 5-aryl-4,6-dithianonanedioic acids (2) as a novel class of selective leukotriene antagonists having potent *in vitro* and *in vivo* activity of considerable duration, in addition to being devoid of agonist activity (Perchonock, McCarthy, Erhard, Gleason, Wasserman, Muccitelli, DeVan, Tucker, Vickery, Kirchner, Weichman, Mong, Crooke & Newton, 1985). In an effort to define the features of these compounds responsible for their biological activity, we sought to obtain structural information on them, particularly with regard to the orientation of the polar head groups and the lipid tail (*R*). NMR data indicated that the methine proton was

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* Author to whom correspondence should be addressed (c/o Department of Analytical, Physical and Structural Chemistry).

† Department of Medicinal Chemistry.

deshielded, suggesting a stable solution conformation in which this proton is close to the plane of the aromatic ring. However, further conformational information on these highly flexible molecules was not forthcoming. We thus turned to the solid state, and report now the crystal structure of a prototypical member of this class, SK&F 102316 [(2), $R = OC_{11}H_{23}$] (Perchonock, Uzinskas, McCarthy, Erhard, Gleason, Wasserman, Muccitelli, DeVan, Tucker, Vickery, Kirchner, Weichman, Mong, Scott, Chi-Rosso, Wu, Crooke & Newton, 1985).

(1)   (2)
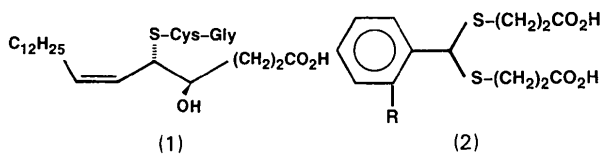
Experimental. Colorless, prismatic single crystals were grown by slow evaporation from acetonitrile. Crystal $0.30 \times 0.30 \times 0.50$ mm mounted in a quartz capillary with longest dimension parallel to φ. Enraf–Nonius CAD-4 diffractometer, graphite monochromator; no systematic absences; cell constants from least-squares analysis of 25 reflections with $30° \leq 2\theta(Mo) \leq 35°$ measured on the diffractometer. Intensity data collected in an ω–θ scan mode, as suggested by peak-shape analysis; 6540 measured intensities, $2\theta \leq 55°$, $-16 \leq h \leq 16$, $-24 \leq k \leq 24$, $0 \leq l \leq 7$; Lorentz–polarization correction, no absorption correction; no systematic fluctuations in reflections $\overline{2}54$, $19\overline{3}$, $\overline{2}93$ monitored at the beginning, end and each 3 h during data collection (34 times); max. deviations in F 3·2, 1·8 and 2·3%, respectively; mean values of F 147·0 (5), 186·6 (6) and 143·8 (4), respectively. Symmetry-equivalent reflections were averaged; agreement factors were 0·016 on I and 0·015 on F_o. Programs in the CAD-4 *SDP*; structure solution from *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980); anisotropic least-squares refinement (on F) of positions led to $wR = 0.114$; weights $4F_o^2/\sigma^2(I)$; subsequent difference Fourier synthesis revealed positions for all H atoms. H atoms allowed to refine in three final least-squares cycles; weighting scheme above with $\sigma(I)$ as defined by Corfield, Doedens & Ibers (1967) with $p = 0.05$, $wR = 0.051$, $S = 1.26$, 3400 observations with $I \geq 3.0\sigma(I)$, 433 variables; extinction parameter included in later stages refined to 8.28 (3) $\times 10^{-7}$; in final least-squares cycles max. $\Delta/\sigma = 0.35$; final difference map was featureless, maximum positive peak height was 0.303 e Å^{-3}. Neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974), for H from Stewart, Davidson & Simpson (1965). Refinement using all data with $I \geq 0.01\sigma(I)$ gave $R = 0.063$.

Discussion. The positional parameters, along with their standard deviations as estimated from the inverse

matrix, are listed in Table 1.* The structure of a single molecule is displayed as Fig. 1. Principal bond lengths and angles are presented in Table 2. In general, there are no unusual bond distances observed in this structure. The S—C distances are of normal length for the atom types involved. There is, however, an apparent asymmetry in the two S—C(7) bond lengths with S(1)—C(7) [1·813 (2) Å] discernibly shorter than its S(2)—C(7) [1·830 (2) Å] counterpart. The S(1)—C(8) and S(2)—C(11) bonds, in contrast, are of equivalent length within the error of the experiment. Bond distances within the phenyl ring range from 1·361 (4) to 1·390 (3) Å and show a normal average of 1·382 (8) Å. Along the undecane chain C—C bond distances range from 1·497 (4) Å for C(14)—C(15) to 1·525 (3) Å for C(15)—C(16) with an average of 1·515 (11) Å. As a whole these distances are shorter than the idealized C_{sp^3}—C_{sp^3} distance of 1·544 Å; however, bond-length shortening due to the thermal motion of the atoms in this straight-chain hydrocarbon moiety is expected in X-ray diffraction results at ambient temperature.

There are some noteworthy adjustments in bond angles around the phenyl ring and its substituent atoms. The angle O(1)—C(2)—C(3) of 124·2 (2)° is widened from 120° and may reflect adjustments to minimize steric interactions between the protons attached to C(14) and the phenyl-ring proton attached at C(3). In addition, the angle C(1)—C(7)—S(2) of 114·1 (2)° is wider than the ideal tetrahedral value and again may reflect adjustments to relieve unfavorable steric interactions between the undecane chain and the thioacetal moiety. Bond angles about the two S atoms show a slight asymmetry with the C(7)—S(2)—C(11) angle of 101·3 (1)° wider than its C(7)—S(1)—C(8) counterpart of 100·9 (1)°. These values are both quite normal for thioether linkages. Phenyl intraring angles show a normal distribution with an average of 120·0 (6)°; the widest angle is 121·0 (3)° at C(6) and the most compressed angle is 118·5 (2)° at C(1).

The phenyl ring is virtually planar with no atom deviating from the six-atom plane by more than 0·022 (2) Å. The two primary substituent atoms O(1) and C(7) sit out of the plane of the phenyl ring on opposite sides with deviations of −0·090 (2) and 0·128 (2) Å, respectively. The best least-squares plane through the eight atoms C(1)—C(7) and O(1) thus shows deviations as large as 0·069 (2) Å.

The proton attached to C(7) also sits out of the six-atom plane by 0·33 (2) Å, in accord with the NMR data. The best least-squares plane through the five atoms O(1)—C(2)—C(1)—C(7)—H(C7) thus shows

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deviations as large as 0·10 (2) Å at H(C7), precluding the assignment of an intramolecular C—H···O hydrogen bond, in agreement with the non-acidic nature of this hydrogen.

The conformations of the undecane and dithioacetal moieties are highly extended. The undecane chain extends away from the phenyl ring in a zigzag *trans* planar conformation. The two thioacetal moieties adopt different conformations and are not parallel as could be implied by two-dimensional representations of this chemical structure. The mercaptopropionate chain at S(1) adopts a full *trans* conformation as indicated by the torsion angles C(1)—C(7)—S(1)—C(8) (−166·5°), C(7)—S(1)—C(8)—C(9) (158·8°) and S(1)—C(8)—C(9)—C(10) (−177·2°). The chain at S(2), in contrast, adopts a *gauche–gauche–trans* conformation as described by the torsion angles C(1)—C(7)—S(2)—C(11) (77·0°), C(7)—S(2)—C(11)—C(12) (70·5°) and S(2)—C(11)—C(12)—C(13) (168·1°) (e.s.d.'s for torsion angles ~0·8°). The best least-squares planes through the six-atom thioacetal moieties are thus inclined at an angle of 47° to one another.

Table 1. *Positional and thermal parameters*

	x	y	z	$B_{eq}^*(Å^2)$
S(1)	0·71815 (5)	0·44472 (3)	0·6750 (1)	3·90 (1)
S(2)	0·85287 (5)	0·30798 (3)	0·9077 (1)	3·83 (1)
O(1)	0·6198 (1)	0·25421 (8)	0·4860 (3)	4·02 (4)
O(2)	0·8739 (2)	0·56357 (9)	0·0961 (4)	5·31 (5)
O(3)	0·9774 (1)	0·45255 (9)	0·2056 (4)	4·91 (4)
O(4)	0·9679 (2)	0·0830 (1)	0·3269 (4)	6·73 (6)
O(5)	0·9589 (2)	0·06341 (9)	0·7093 (4)	6·62 (6)
C(1)	0·6256 (2)	0·3459 (1)	0·7896 (4)	3·09 (5)
C(2)	0·5693 (2)	0·3000 (1)	0·6681 (4)	3·27 (5)
C(3)	0·4697 (2)	0·3015 (1)	0·7354 (5)	4·21 (6)
C(4)	0·4277 (2)	0·3474 (1)	0·9275 (5)	4·97 (7)
C(5)	0·4842 (2)	0·3901 (1)	1·0571 (5)	4·95 (7)
C(6)	0·5829 (2)	0·3897 (1)	0·9881 (5)	4·14 (6)
C(7)	0·7290 (2)	0·3492 (1)	0·7023 (4)	3·06 (5)
C(8)	0·8305 (2)	0·4358 (1)	0·5010 (5)	3·77 (5)
C(9)	0·8104 (2)	0·5067 (1)	0·3786 (5)	3·99 (6)
C(10)	0·8957 (2)	0·5042 (1)	0·2198 (5)	3·75 (5)
C(11)	0·8730 (2)	0·2117 (1)	0·8366 (5)	3·72 (6)
C(12)	0·9083 (2)	0·1865 (1)	0·5860 (5)	3·81 (6)
C(13)	0·9470 (2)	0·1048 (1)	0·5476 (5)	3·92 (6)
C(14)	0·5668 (2)	0·2055 (1)	0·3501 (5)	3·76 (5)
C(15)	0·6445 (2)	0·1605 (1)	0·1784 (5)	4·17 (6)
C(16)	0·5990 (2)	0·1079 (1)	0·0065 (5)	4·13 (6)
C(17)	0·6834 (2)	0·0598 (1)	−0·1510 (5)	4·56 (6)
C(18)	0·6420 (2)	0·0081 (1)	−0·3345 (5)	4·29 (6)
C(19)	0·7286 (2)	−0·0404 (1)	−0·4833 (5)	4·75 (7)
C(20)	0·6902 (2)	−0·0917 (1)	−0·6752 (5)	4·40 (6)
C(21)	0·7804 (2)	−0·1414 (1)	−0·8128 (5)	4·65 (7)
C(22)	0·7453 (2)	−0·1924 (1)	−1·0102 (5)	4·39 (6)
C(23)	0·8393 (2)	−0·2423 (2)	−1·1377 (6)	5·42 (8)
C(24)	0·8057 (3)	−0·2914 (2)	−1·3406 (6)	6·11 (9)

$^* B_{eq} = \frac{4}{3}[a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + ab(\cos\gamma)\beta_{12} + ac(\cos\beta)\beta_{13} + bc(\cos\alpha)\beta_{23}].$
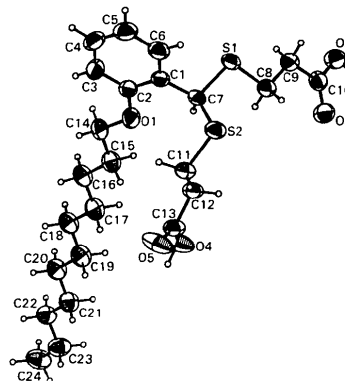

Fig. 1. View of the 5-(2-undecyloxyphenyl)-4,6-dithianonanedioic acid molecule showing the labeling scheme employed. Thermal ellipsoids are drawn at the 50% probability level; H atoms are shown as small spheres of arbitrary size.

Table 2. *Principal bond distances (Å) and angles (°)*

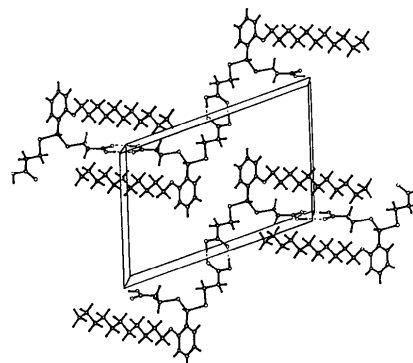|			
S(1)—C(7)	1·813 (2)	S(1)—C(8)	1·810 (2)
S(2)—C(7)	1·830 (2)	S(2)—C(11)	1·803 (2)
O(1)—C(2)	1·372 (3)	O(1)—C(14)	1·432 (3)
O(2)—C(10)	1·312 (3)	O(3)—C(10)	1·212 (3)
O(4)—C(13)	1·289 (3)	O(5)—C(13)	1·205 (3)
C(1)—C(2)	1·390 (3)	C(1)—C(6)	1·390 (3)
C(1)—C(7)	1·508 (3)	C(2)—C(3)	1·385 (3)
C(3)—C(4)	1·378 (4)	C(4)—C(5)	1·361 (4)
C(5)—C(6)	1·385 (4)	C(8)—C(9)	1·505 (3)
C(9)—C(10)	1·490 (3)	C(11)—C(12)	1·508 (3)
C(12)—C(13)	1·498 (3)	C(14)—C(15)	1·497 (4)
C(15)—C(16)	1·525 (3)	C(16)—C(17)	1·517 (4)
C(17)—C(18)	1·521 (3)	C(18)—C(19)	1·509 (4)
C(19)—C(20)	1·524 (4)	C(20)—C(21)	1·511 (4)
C(21)—C(22)	1·522 (3)	C(22)—C(23)	1·515 (4)
C(23)—C(24)	1·507 (4)		
C(7)—S(1)—C(8)	100·9 (1)	O(2)—C(10)—O(3)	123·0 (2)
C(7)—S(2)—C(11)	101·3 (1)	O(2)—C(10)—C(9)	113·3 (2)
C(2)—O(1)—C(14)	119·2 (2)	O(3)—C(10)—C(9)	123·7 (2)
C(2)—C(1)—C(6)	118·5 (2)	S(2)—C(11)—C(12)	113·8 (2)
C(2)—C(1)—C(7)	120·3 (2)	C(11)—C(12)—C(13)	113·5 (2)
C(6)—C(1)—C(7)	121·2 (2)	O(4)—C(13)—O(5)	123·3 (2)
O(1)—C(2)—C(1)	115·6 (2)	O(4)—C(13)—C(12)	113·7 (2)
O(1)—C(2)—C(3)	124·2 (2)	O(5)—C(13)—C(12)	123·0 (2)
C(1)—C(2)—C(3)	120·2 (2)	O(1)—C(14)—C(15)	106·2 (2)
C(2)—C(3)—C(4)	119·9 (3)	C(14)—C(15)—C(16)	113·8 (2)
C(3)—C(4)—C(5)	120·9 (3)	C(15)—C(16)—C(17)	111·8 (2)
C(4)—C(5)—C(6)	119·5 (3)	C(16)—C(17)—C(18)	114·5 (2)
C(1)—C(6)—C(5)	121·0 (3)	C(17)—C(18)—C(19)	113·3 (2)
S(1)—C(7)—S(2)	108·0 (1)	C(18)—C(19)—C(20)	115·2 (2)
S(1)—C(7)—C(1)	108·3 (1)	C(19)—C(20)—C(21)	113·5 (2)
S(2)—C(7)—C(1)	114·1 (2)	C(20)—C(21)—C(22)	115·3 (2)
S(1)—C(8)—C(9)	108·5 (2)	C(21)—C(22)—C(23)	113·1 (2)
C(8)—C(9)—C(10)	113·1 (2)	C(22)—C(23)—C(24)	114·0 (3)

Fig. 2. View of the unit-cell packing in the 5-(2-undecyloxyphenyl)-4,6-dithianonanedioic acid structure. Dashed lines indicate hydrogen bonds.

A diagram of a portion of the unit-cell packing is presented as Fig. 2. There is a distinct separation of hydrophobic and hydrophilic groups within the crystal. Nonbonded hydrophobic interactions between adjacent undecane chains undoubtedly contribute to crystal stabilization. In addition, there are two strong intermolecular hydrogen bonds involving both carboxyl groups interacting in a dimeric fashion across crystallographic inversion centers. The associated metrical parameters are $O(2)\cdots O(3) = 2\cdot648$ (2), $H1(O2)\cdots O(3) = 1\cdot67$ (3) Å, $O(2)-H1(O2)\cdots O(3) = 170$ (3)°, $O(4)\cdots O(5) = 2\cdot673$ (3), $H1(O4)\cdots O(5) = 1\cdot81$ (4) Å and $O(4)-H1(O4)\cdots O(5) = 176$ (3)°.

References

CORFIELD, P. W. R., DOEDENS, R. J. & IBERS, J. A. (1967). *Inorg. Chem.* **6**, 197–204.

DAHLEN, S. E., HANSSON, G., HEDQUIST, P., BJORCK, T., GRANSTROM, E. & DAHLEN, B. (1983). *Proc. Natl Acad. Sci. USA*, **80**, 1712–1716.

DAHLEN, S. E., HEDQUIST, P., HAMMERSTROM, S. & SAMUELSON, B. (1980). *Nature (London)*, **288**, 484–486.

GLEASON, J. G., KU, T. W., MCCARTHY, M. E., WEICHMAN, B. M., HOLDEN, D. A., OSBORN, R. R., ZABKO-POTAPOVICH, B., BERKOWITZ, B. & WASSERMAN, M. A. (1983). *Biochem. Biophys. Res. Commun.* **117**, 732–739.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

KU, T. W., MCCARTHY, M. E., WEICHMAN, B. M. & GLEASON, J. G. (1985). *J. Med. Chem.* Submitted.

LEWIS, R. A., AUSTEN, K. F., DRAZEN, J. M., CLARK, D. A., MARFAT, A. & COREY, E. J. (1980). *Proc. Natl Acad. Sci. USA*, **77**, 3710–3714.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain. Belgium.

MAROM, Z., SHELHAMER, J. H., BACH, M. K., MORTON, D. R. & KALINER, M. (1982). *Am. Rev. Respir. Dis.* **126**, 449–451.

PECK, M. J., PIPER, P. G. & WILLIAMS, T. J. (1981). *Prostaglandins*, **21**, 315–321.

PERCHONOCK, C. D., MCCARTHY, M. E., ERHARD, K. F., GLEASON, J. G., WASSERMAN, M. A., MUCCITELLI, R. M., DEVAN, J. F., TUCKER, S. S., VICKERY, L. M., KIRCHNER, T., WEICHMAN, B. M., MONG, S., CROOKE, S. T. & NEWTON, J. F. (1985). *J. Med. Chem.* **28**, 1145–1147.

PERCHONOCK, C. D., UZINSKAS, I., KU, T. W., MCCARTHY, M. E., BONDINELL, W. E., VOLPE, B. W., GLEASON, J. G., WEICHMAN, B. M., MUCCITELLI, R. M., DEVAN, J. F., TUCKER, S. S., VICKERY, L. M. & WASSERMAN, M. A. (1985). *Prostaglandins*, **29**, 75–81.

PERCHONOCK, C. D., UZINSKAS, I., MCCARTHY, M. E., ERHARD, K. F., GLEASON, J. G., WASSERMAN, M. A., MUCCITELLI, R. M., DEVAN, J. F., TUCKER, S. S., VICKERY, L. M., KIRCHNER, T., WEICHMAN, B. M., MONG, S., SCOTT, M. O., CHI-ROSSO, G., WU, H.-L. W., CROOKE, S. T. & NEWTON, J. F. (1985). *J. Med. Chem.* Submitted.

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

WEICHMAN, B. M., WASSERMAN, M. A., HOLDEN, D. A., OSBORN, R. R., WOODWARD, D. F., KU, T. W. & GLEASON, J. G. (1983). *J. Pharmacol. Exp. Ther.* **227**, 700–705.

WOODWARD, D. F., WEICHMAN, B. M., GILL, C. A. & WASSERMAN, M. A. (1983). *Prostaglandins*, **25**, 131–142.

Structure of Antischistosome Compounds. I. (2-Aminoethyl)triphenylphosphonium Bromide Hydrobromide

BY EDMUND W. CZERWINSKI

Division of Biochemistry, Department of Human Biological Chemistry and Genetics, The University of Texas Medical Branch, Galveston, Texas 77550, USA

Abstract. $C_{20}H_{22}NP^{2+}.2Br^-$, $M_r = 467\cdot2$, orthorhombic, $P2_12_12_1$, $a = 9\cdot262$ (2), $b = 12\cdot846$ (2), $c = 16\cdot845$ (3) Å, $V = 2004\cdot2$ (2) Å^3, $Z = 4$, $D_x = 1\cdot548$ g cm^{-3}, graphite-monochromated Cu $K\bar{\alpha}$ radiation, $\lambda = 1\cdot5418$ Å, $\mu = 59\cdot45$ cm^{-1}, $F(000) = 936$, $T = 292$ K, $R = 0\cdot034$ and $wR = 0\cdot035$ for 2158 unique reflections with $I > 3\sigma(I)$. The structure contains two non-bonded bromide ions and a divalent tetrahedral (aminoethyl)triphenylphosphonium cation. The four P—C distances are in the range $1\cdot790$ (4)–$1\cdot798$ (5) Å with a mean of $1\cdot795$ (3) Å. The six C—P—C angles range from $107\cdot5$ (2) to $111\cdot3$ (2)°. The aminoethyl group is extended with torsion angles of $-161\cdot1$ (3)° for P—C—C—N and $-175\cdot2$ (3), $-56\cdot6$ (6) and $66\cdot7$ (6)° for the C—P—C—C angles. The closest phosphorus–bromine distance is $4\cdot580$ (1) Å. The ammonium ion moiety interacts with four bromide ions to form a network which disperses and neutralizes the charges.

Introduction. The title compound is one of a series of alkyl-, alkylamino- and poly(methylene)bis(triphenylphosphonium) compounds which exhibit varying effects on the cholinergic nervous system of *Schistosoma mansoni* (McAllister, Dotson, Grim & Hillman, 1980). The biological effects of these compounds cannot be