approximations, this approach was successful in rationalizing the rigid systems like coumarin derivatives (Murthy, Arjunan, Venkatesan & Ramamurthy, 1986). We have assumed in these calculations that the overall topography of the excited molecule is the same as in the ground state. This clearly is not true and this assumption is more serious in the present molecule than in rigid molecules such as coumarins. In its reaction pathway involving change in the hybridization of the reactive atoms C(9) and C(14) from sp^2 to sp^3 with a lengthy styrene side group at C(9), it would be expected that the side group undergoes considerable positional changes in the existing crystal lattice which might not be favourable from the intermolecular energy calculations. It seems most likely that the available cavity volume (Cohen, 1975) is insufficient as the molecular topology undergoes very large changes in the course of the reaction path from the reactant to the product.

We record our grateful thanks to Professor A. J. Birch, FRS, Australian Academy of Sciences, for suggesting this problem and Professor V. Ramakrishnan for useful discussions.

References

ARIEL, S., ASKARI, S., SCHEFFER, J. R., TROTTER, J. & WALSH, L. (1984). *J. Am. Chem. Soc.* **106**, 5726–5728.

BHADBHADE, M. M., MURTHY, G. S., VENKATESAN, K. & RAMAMURTHY, V. (1984). *Chem. Phys. Lett.* **109**, 259–263.

BUSING, W. R. (1981). *WMIN*. A computer program to model molecules and crystals in terms of potential-energy functions. Report ORNL-5747. Oak Ridge National Laboratory, Tennessee.

COHEN, M. D. (1975). *Angew. Chem. Int. Ed. Engl.* **14**, 386–393.

COHEN, M. D. & SCHMIDT, G. M. J. (1964). *J. Chem. Soc.* pp. 1996–1999.

COHEN, M. D., SCHMIDT, G. M. J. & SONNTAG, F. J. (1964). *J. Chem. Soc.* pp. 2000–2013.

GNANAGURU, K., RAMASUBBU, N., VENKATESAN, K. & RAMAMURTHY, V. (1985). *J. Org. Chem.* **50**, 2337–2346.

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

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.

MIRSKY, K. (1978). In *Computing in Crystallography*, edited by H. SCHENK, R. OLITHOF-HAZEKAMP, H. VAN KONINGSVELD & G. C. BASSI, pp. 169–182. Delft Univ. Press.

MURTHY, G. S., ARJUNAN, P., VENKATESAN, K. & RAMAMURTHY, V. (1986). *Tetrahedron*. In the press.

NAKANISHI, H., PARKINSON, G. M., JONES, W., THOMAS, J. M. & HASEGAWA, M. (1979). *Isr. J. Chem.* **18**, 261–265.

RAMAMURTHY, V. & VENKATESAN, K. (1986). *Chem. Rev.* In the press.

READ, J. & SMITH, H. G. (1921). *J. Chem. Soc.* **119**, 779–789.

READ, J. & SMITH, H. G. (1922). *J. Chem. Soc.* **121**, 574–593.

ROMERS, C., ALTONA, C., BUYS, H. R. & HAVINGA, E. (1969). In *Topics in Sterochemistry*, Vol. 4, edited by E. L. ELIEL & N. L. ALLINGER, pp. 39–98. New York: John Wiley.

SCHMIDT, G. M. J. (1964). *J. Chem. Soc.* pp. 2014–2021.

SHELDRICK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

Acta Cryst. (1987). C**43**, 1131–1134

Structure of 5-(*p*-Aminobenzenesulfonamido)-1-phenylpyrazole (Sulfaphenazole)*

BY H. C. PATEL AND T. P. SINGH

Department of Biophysics, All-India Institute of Medical Sciences, New Delhi – 110029, India

(*Received* 25 *August* 1986; *accepted* 12 *January* 1987)

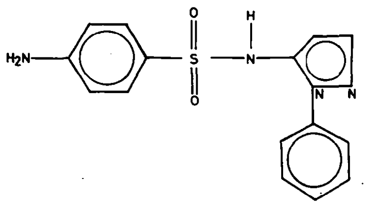
Abstract. $C_{15}H_{14}N_4O_2S$, M_r=314·4, monoclinic, $P2_1/n$, a = 14·760 (3), b = 11·253 (2), c = 19·213 (4) Å, β = 109·90 (3)°, V = 3001 (1) Å^3, Z = 8, D_m = 1·397 (5), D_x = 1·3916 (5) Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ = 0·216 mm^{-1}, F(000) = 1312, T = 293 K, final R = 0·067 for 3208 observed reflections. The two crystallographically independent molecules A and B in the structure have similar molecular dimensions but their conformations are substantially different. The six-membered benzene-ring planes in molecule A and in molecule B are inclined to the planar pyrazole rings at 53·5 (4) and 46·9 (4)°; 75·9 (3) and 69·1 (4)° respectively. The two benzene-ring planes in molecule A are mutually inclined at 12·8 (3)° while those in molecule B are oriented at 36·5 (4)°. Both molecules show *gauche* conformations about the S—N bonds with torsion angles of −73·7 (8) and 94·0 (8)° respectively. The molecules are packed in the form of hydrogen-bonded helices which are interconnected by hydrogen bonds and van der Waals forces through the amino N atoms and the sulfonyl O atoms.

---

* *Chemical Abstracts* name: 4-amino-*N*-(1-phenyl-1*H*-pyrazol-5-yl)benzenesulfonamide.

0108-2701/87/061131-04$01.50

Introduction. Sulfonamides are well known antibacterial agents. They produce antimicrobial effects by competitively inhibiting the enzyme dihydropteroate synthase (DHPS) towards the substrate *p*-aminobenzoic acid (PABA) (Bock, Miller, Schaper & Seydel, 1974). As part of our programme of systematic studies on sulfonamides and the enzyme DHPS (Haridas & Singh, 1986), we report here the crystal structure of sulfaphenazole (I).



(I)

Experimental. Samples of sulfaphenazole obtained directly from the market in the form of 'orisul' tablets, crystallized from solution in methanol at 293 K. Large, pyramidal and colourless crystals: one $1{\cdot}00 \times 0{\cdot}60 \times 0{\cdot}50$ mm used for data collection. Unit-cell dimensions and space group from oscillation and Weissenberg photographs. Cell dimensions refined from 15 independent reflections (θ range: 4·0 to 20·0°) on diffractometer. Density by flotation in benzene and carbon tetrachloride. Intensity data collected on Enraf–Nonius CAD-4 automatic four-circle diffractometer in ω–2θ scan mode using graphite-monochromated Mo $K\alpha$ radiation. Total number of reflections measured 4007, total number of independent reflections 3208 ($I \geq 2\sigma$) for $(\sin\theta)/\lambda \leq 0{\cdot}54$ Å^{-1} with $h = -15$ to 14, $k = 0$ to 12, $l = 0$ to 20. Corrections for Lorentz and polarization effects but not for absorption ($\mu r = 0{\cdot}119$). Intensity measurements of two standard reflections (400 and 004) repeated after every 50 reflections. Variations in intensity throughout the experiment $\leq 5{\cdot}3\%$, $R_{\rm int}$ (for merged data) = 4·2%. Structure solved by *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and refined by block-diagonal structure factor least-squares procedure. Positions of H atoms from difference Fourier map. Non-hydrogen atoms refined anisotropically and H atoms isotropically. Final R for 3208 observed reflections = 0·067, $wR = 0{\cdot}087$, $S = 0{\cdot}97$. Final $\Delta\rho$ excursions −0·15 to 0·14 e Å^{-3} and $(\Delta/\sigma)_{\max} = 0{\cdot}096$. Weighting function $w = 1/(0{\cdot}50 + 0{\cdot}0655|F_o| + 0{\cdot}0005|F_o|^2)$ (Cruickshank, 1961*a*) adjusted to make the average independent of F_o. $\sum w(\Delta F)^2$ used in the block-diagonal least-squares refinement. *SFLS* program originally written by Shiono (1968/1971) and extensively modified by the authors. Atomic scattering factors for S from *International Tables for X-ray Crystallography* (1962), for C, N, O from Cromer & Mann (1968) and for H from Stewart, Davidson & Simpson (1965). All calculations on the HP computers at the All-India Institute of Medical Sciences, New Delhi.

Table 1. *Fractional coordinates* (×10⁴) *of the non-hydrogen atoms and equivalent isotropic thermal parameters* (×10⁴)

$$B_{\rm eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j B_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$(Å^2)
C1	992 (7)	3694 (9)	6397 (5)	37 (4)
C2	1933 (7)	3672 (9)	6870 (6)	42 (4)
C3	2523 (7)	4628 (10)	6914 (6)	49 (4)
C4	2190 (8)	5644 (10)	6492 (5)	52 (4)
C5	1226 (9)	5654 (11)	6017 (6)	59 (5)
C6	648 (8)	4703 (10)	5977 (6)	51 (5)
N7	2759 (8)	6612 (10)	6541 (6)	79 (5)
S8	201 (2)	2505 (2)	6328 (1)	28 (1)
O9	704 (5)	1562 (6)	6794 (4)	44 (3)
O10	−309 (6)	2271 (7)	5562 (4)	54 (3)
N11	−620 (5)	2965 (7)	6655 (4)	37 (3)
C12	−390 (6)	3114 (8)	7420 (5)	36 (3)
C13	204 (7)	3893 (9)	7920 (6)	50 (4)
C14	174 (7)	3539 (9)	8602 (5)	48 (4)
N15	−382 (6)	2599 (7)	8547 (4)	44 (3)
N16	−725 (5)	2336 (6)	7814 (4)	38 (2)
C17	−1366 (6)	1364 (7)	7560 (4)	35 (3)
C18	−1145 (7)	299 (8)	7927 (5)	42 (3)
C19	−1762 (8)	−642 (9)	7701 (6)	55 (4)
C20	−2604 (8)	−523 (10)	7098 (6)	58 (4)
C21	−2832 (7)	561 (9)	6737 (5)	42 (4)
C22	−2213 (6)	1513 (8)	6962 (5)	36 (3)
C23	3562 (6)	1497 (8)	5583 (4)	37 (3)
C24	3244 (7)	1577 (8)	6175 (5)	42 (3)
C25	2562 (7)	802 (9)	6248 (5)	43 (4)
C26	2173 (7)	−64 (9)	5710 (6)	47 (4)
C27	2506 (8)	−140 (9)	5112 (6)	56 (4)
C28	3191 (7)	629 (9)	5054 (5)	47 (4)
N29	1495 (8)	−848 (10)	5787 (6)	72 (5)
S30	4416 (2)	2494 (2)	5480 (1)	26 (1)
O31	4670 (5)	3285 (6)	6092 (3)	57 (3)
O32	5139 (5)	1832 (7)	5315 (4)	35 (3)
N33	3860 (5)	3250 (7)	4723 (4)	35 (3)
C34	3410 (6)	4343 (8)	4718 (4)	35 (3)
C35	3769 (7)	5422 (9)	4990 (5)	43 (4)
C36	2999 (8)	6199 (9)	4761 (6)	54 (4)
N37	2192 (6)	5650 (8)	4362 (5)	46 (3)
N38	2447 (5)	4499 (7)	4351 (4)	38 (3)
C39	1728 (6)	3634 (9)	4003 (5)	37 (3)
C40	1461 (8)	2820 (12)	4427 (7)	49 (5)
C41	766 (9)	1998 (14)	4095 (9)	68 (6)
C42	333 (9)	1993 (14)	3332 (9)	77 (6)
C43	603 (9)	2812 (16)	2918 (7)	65 (7)
C44	1305 (8)	3637 (12)	3249 (6)	50 (5)

Discussion. There are two molecules of sulfaphenazole in the asymmetric unit. The final positional and equivalent isotropic temperature factors of non-hydrogen atoms are given in Table 1.* The bond lengths and valence angles involving non-hydrogen atoms are listed in Table 2. The perspective view with the numbering scheme of the crystallographically independent molecules A and B is illustrated in Fig. 1. The crystal structure and the hydrogen-bonding scheme are shown in Fig. 2. The average C—H and N—H

---

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, torsion angles, least-squares-planes data and intermolecular contact distances have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43719 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

distances are 0·99 (10) and 0·85 (11) Å respectively. The bond lengths and angles involving non-hydrogen atoms are comparable to those found in other sulfonamides (Haridas & Singh, 1987). The molecules *A* and *B* are nearly the same except for the angle S—N—C which is 119·8 (7) in molecule *A* but 123·7 (6)° in molecule *B*. Bonds around S atoms are distorted from the ideal tetrahedral geometry, the angles around S varying from 104·8 (5) to 119·2 (5)° in molecule *A* and from 105·7 (4) to 120·4 (5)° in *B*. These deviations result from the steric hindrance of dissimilar groups and from the type of non-bonded interactions described by Bartell (1962). The shortening of bond distances around S atoms (Table 2) indicates a substantial amount of double-bond character. Abrahams (1955) has calculated the S—C single-bond distance to be 1·82 Å, which is close to the sum of the Pauling (1960) covalent radii for S and C. Schomaker & Stevenson (1941) have estimated the S—N single-bond distance to be 1·74 Å while in sulfamic acid (Sass, 1960) where the N atom has no orbital available for π-bonding, the S—N link is 1·76 (2) Å. Cruickshank (1961*b*) has assigned bond orders of about 0·66 for S—O bonds in the region of 1·43 Å. Furthermore, the S—O distances in molecules *A* and *B* are the same though both O atoms of *A* are hydrogen-bonded while those of *B* are not. This agrees well with our earlier conclusion that S—O distances do not vary as a result of interaction through them (Haridas & Singh, 1987). The distances in the pyrazole moieties lie typically between the corresponding single- and double-bond distances. The benzene rings in molecule *A* are rotated with respect to each other at 12·8 (3)° while those in *B* are oriented at

Table 2. *Bond lengths* (Å) *and bond angles* (°) *involving non-hydrogen atoms*

C1–C2	1·377 (12)	C23–C24	1·373 (13)
C1–C6	1·386 (14)	C23–C28	1·382 (12)
C1–S8	1·751 (10)	C23–S30	1·748 (10)
C2–C3	1·369 (15)	C24–C25	1·375 (15)
C3–C4	1·390 (14)	C25–C26	1·394 (13)
C4–C5	1·406 (14)	C26–C27	1·398 (16)
C4–N7	1·359 (16)	C26–N29	1·379 (16)
C5–C6	1·354 (17)	C27–C28	1·365 (16)
S8–O9	1·423 (7)	S30–O31	1·420 (7)
S8–O10	1·431 (6)	S30–O32	1·424 (8)
S8–N11	1·626 (9)	S30–N33	1·644 (6)
N11–C12	1·401 (11)	N33–C34	1·396 (12)
C12–C13	1·374 (12)	C34–C35	1·357 (13)
C12–N16	1·357 (12)	C34–N38	1·367 (16)
C13–C14	1·385 (15)	C35–C36	1·382 (14)
C14–N15	1·320 (13)	C36–N37	1·329 (12)
N15–N16	1·357 (9)	N37–N38	1·351 (12)
N16–C17	1·419 (10)	N38–C39	1·427 (11)
C17–C18	1·373 (12)	C39–C40	1·370 (17)
C17–C22	1·391 (10)	C39–C44	1·368 (12)
C18–C19	1·367 (14)	C40–C41	1·367 (18)
C19–C20	1·387 (14)	C41–C42	1·385 (21)
C20–C21	1·387 (14)	C42–C43	1·364 (23)
C21–C22	1·378 (13)	C43–C44	1·376 (19)

C2–C1–C6	119·1 (9)	C24–C23–C28	119·7 (8)
C2–C1–S8	122·2 (7)	C24–C23–S30	121·0 (7)
C6–C1–S8	118·7 (7)	C28–C23–S30	119·4 (7)
C3–C2–C1	120·3 (9)	C25–C24–C23	120·7 (9)
C2–C3–C4	121 (1)	C24–C25–C26	120 (1)
N7–C4–C3	122 (1)	N29–C26–C25	120 (1)
N7–C4–C5	120 (1)	N29–C26–C27	121 (1)
C3–C4–C5	118 (1)	C25–C26–C27	118·7 (9)
C6–C5–C4	121 (1)	C28–C27–C26	120 (1)
C5–C6–C1	121 (1)	C27–C28–C23	120·5 (9)
O9–S8–O10	119·2 (4)	O31–S30–O32	120·4 (4)
O9–S8–N11	107·1 (4)	O31–S30–N33	108·7 (4)
O9–S8–C1	109·3 (4)	O31–S30–C23	107·8 (4)
O10–S8–N11	104·8 (4)	O32–S30–N33	105·0 (4)
O10–S8–C1	108·8 (4)	O32–S30–C23	108·3 (4)
N11–S8–C1	107·0 (4)	N33–S30–C23	105·7 (4)
S8–N11–C12	119·8 (6)	S30–N33–C34	123·7 (6)
N16–C12–C13	106·7 (8)	N38–C34–C35	106·5 (8)
N16–C12–N11	120·3 (8)	N38–C34–N33	121·7 (7)
C13–C12–N11	132·8 (8)	C35–C34–N33	131·6 (8)
C12–C13–C14	105·1 (9)	C34–C35–C36	105·8 (9)
N15–C14–C13	111·7 (9)	N37–C36–C35	111·6 (9)
C14–N15–N16	105·2 (8)	C36–N37–N38	104·8 (4)
C12–N16–N15	111·1 (7)	C34–N38–N37	111·2 (7)
C12–N16–C17	129·2 (7)	C34–N38–C39	129·1 (7)
N15–N16–C17	119·7 (7)	N37–N38–C39	119·6 (7)
C18–C17–C22	121·3 (8)	C44–C39–C40	121 (1)
C18–C17–N16	118·8 (8)	C40–C39–N38	119·7 (9)
C22–C17–N16	119·9 (7)	C44–C39–N38	119·6 (9)
C19–C18–C17	119·8 (9)	C41–C40–C39	120 (1)
C18–C19–C20	120 (1)	C40–C41–C42	120 (1)
C21–C20–C19	120 (1)	C43–C42–C41	120 (1)
C22–C21–C20	120·3 (9)	C42–C43–C44	121 (1)
C21–C22–C17	118·7 (8)	C39–C44–C43	119 (1)

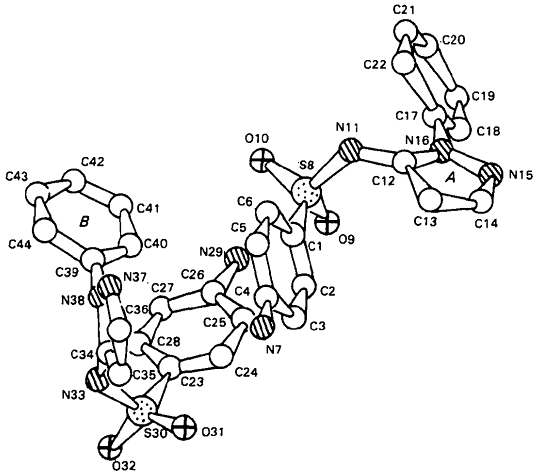


Fig. 1. A perspective view of the molecules as seen down the *b* axis and the numbering scheme.

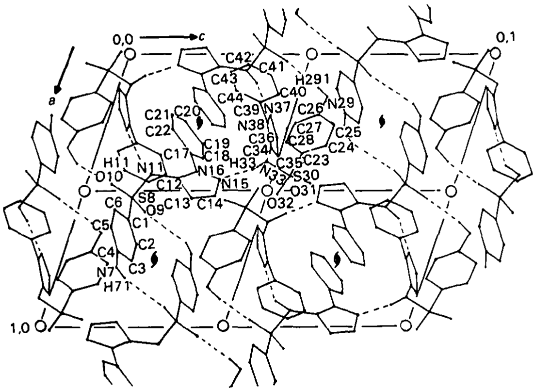


Fig. 2. The crystal structure as viewed along the *b* axis. The dashed lines indicate the hydrogen bonds.

36·5 (4)°. The planes of the benzene rings of the sulfonilamide moieties in molecules *A* and *B* are inclined with respect to the planes of the pyrazole rings at 53·5 (4) and 75·9 (3)° respectively. The planes of benzene rings and the pyrazole rings in molecules *A* and *B* are rotated with respect to each other by 46·9 (4) and 69·1 (4)° respectively. As has been observed in other sulfonamides (Haridas & Singh, 1987), both molecules adopt *gauche* conformations about the S—N bonds with torsion angles of −73·7 (8) and 94·0 (8)° respectively. The torsion angle S(8)—N(11)—C(12)—N(16) is −107·1 (9)° in molecule *A* while the corresponding angle in *B* is −119·7 (8)°. As has been described above, it is clear that the two crystallographically independent molecules have identical molecular dimensions but substantially different conformations. This shows that sulfaphenazole is a flexible molecule capable of undergoing conformational change as a result of variation in the intermolecular interactions while the molecular dimensions remain unchanged.

Molecular packing and hydrogen bonding. The crystal structure as seen down the *b* axis is shown in Fig. 2. The molecules are packed rather compactly and form hydrogen-bonded helices along the screw axes. These helices are formed as a result of N—H···N-type hydrogen bonds involving the imino nitrogen atoms N(11) and N(33) as proton donors and the hetero-nitrogen atoms N(37) and N(15) of the five-membered rings as the corresponding acceptors. The interior of the helix is filled with screw-related benzene rings. The sulfonilamide moieties are disposed outwardly from the helix and provide the interhelix linkage through hydrogen bonds and van der Waals forces. The amino nitrogen atoms N(7) and N(29) form hydrogen bonds with O(9) and O(10) respectively. The sulfonyl oxygen atoms O(31) and O(32) of molecule *B* form van der Waals contacts with C(18), C(19) and C(14), N(15) respectively. It is observed that the two crystallographically independent molecules *A* and *B* are involved in different types of intermolecular interactions and hence exhibit conformational variability, thus showing the flexible nature of the sulfaphenazole molecule. This might mean that this molecule is adaptable to the variable stereochemical receptor site.

The authors gratefully acknowledge financial support from ICMR, New Delhi.

References

Abrahams, S. C. (1955). *Acta Cryst.* **8**, 661–691.

Bartell, L. S. (1962). *Tetrahedron*, **17**, 17.

Bock, L., Miller, G. H., Schaper, K. J. & Seydel, J. K. (1974). *J. Med. Chem.* **17**, 23–28.

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

Cruickshank, D. W. J. (1961*a*). In *Computing Methods and the Phase Problem in X-ray Crystal Structure Analysis*, edited by R. Pepinsky, pp. 32–62. Oxford: Pergamon.

Cruickshank, D. W. J. (1961*b*). *J. Chem. Soc.* pp. 5486–5504.

Haridas, M. & Singh, T. P. (1986). *Ind. J. Chem.* **25**A, 707–713.

Haridas, M. & Singh, T. P. (1987). *Ind. J. Biochem. Biophys.* In the press.

International Tables for X-ray Crystallography (1962). Vol. II, pp. 202–203. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G. Declercq, J.-P. & Woolfson, M. M. (1980). *MULTAN*80. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.

Pauling, L. (1960). *The Nature of the Chemical Bond*. Ithaca, New York: Cornell Univ. Press.

Sass, R. L. (1960). *Acta Cryst.* **13**, 320–324.

Schomaker, V. & Stevenson, D. P. (1941). *J. Am. Chem. Soc.* **63**, 39–40.

Shiono, R. (1968/1971). *SFLS*. Tech. Reps. 48 and 49. Crystallography Laboratory, Univ. of Pittsburgh.

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

Acta Cryst. (1987). C**43**, 1134–1138

Structure and Molecular-Packing Analysis of a Heptofuranosoimidazolidine-2-thione*

By M. D. Estrada, A. Conde and R. Márquez

Departamento de Física del Estado Sólido, Facultad de Física, Universidad de Sevilla, Spain

(*Received* 13 *June* 1986; *accepted* 6 *January* 1987)

Abstract. 1-(4-Bromophenyl)-3-ethyl-(3,5,6,7-tetra-*O*-acetyl-1,2-dideoxy-D-*glycero*-*β*-D-*talo*-heptofuranoso)-[2,1-*d*]imidazolidine-2-thione, $C_{24}H_{29}BrN_2O_9S$, $M_r =$ 601·46, orthorhombic, $P2_12_12_1$, $a = 15{\cdot}634$ (3), $b = 22{\cdot}749$ (6), $c = 7{\cdot}714$ (2) Å, $V = 2743$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}46$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 1{\cdot}60$ mm^{-1}, $F(000) = 1240$, room temperature, final $wR = 0{\cdot}052$ for 1643 observed reflexions.

---

* IUPAC name: 1-{6-acetoxy-3-bromophenyl-2-thioxo-2,3,3a,-5,6,6a-tetrahydro-1*H*-furo[2,3-*d*]imidazol-5-yl}propane-1,2,3-triyl triacetate.