in intensity. 2675 observed reflections with $I \geq 2\sigma(I)$. Structure solved by Patterson analysis, refined by full-matrix least squares, $\sum w(|F_o| - |F_c|)^2$ minimized, anisotropic thermal parameters for non-H atoms. All H atoms located in difference Fourier synthesis and positional parameters included in further refinement with fixed isotropic temperature factor. Final $R =$ 0·073, $R_w = 0\cdot080$; empirical weighting scheme giving no trends in $\langle w\Delta^2 F \rangle$. No correction for absorption. No significant features in final ΔF synthesis. Max. Δ/σ = 0·06. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Calculations performed with *XRAY*70 (Stewart, Kundell & Baldwin, 1970), programs *PARST* (Nardelli, 1982) and *PESOS* (Martínez-Ripoll & Cano, 1975) on a Univac 1108 computer.

Discussion. The structure of the title compound with the atomic numbering is shown in Fig. 1 (*ORTEP*; Johnson, 1965). Positional parameters and the equivalent U values of the anisotropic temperature factor are given in Table 1. Bond lengths and angles and torsion angles are given in Table 2.*

Bond distances are in good agreement with those found in the literature and with other pyridinium iodides previously reported (Smith-Verdier, Florencio & García-Blanco, 1983).

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and deviations from the molecular plane have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39705 (46 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The average torsion angles in the A,B,C and pyridine rings are 2·2 (18), 2·8 (20), 0·8 (20) and 2·9 (16)°, respectively. The torsion angles around the C(1)–C(7), C(3)–C(19) and C(5)–C(13) bonds are 55·1 (14), 25·5 (14) and 57·0 (14)°, respectively. Consequently, there is no electronic interaction in the molecule and the positive charge is localized on the N atom.

The environment of the I^- ion is approximately tetrahedral with I···N distances about 4·6 Å. The nearest contacts between the molecule and the un-attached I^- ion are I···Cl $(x, y, z) = 3\cdot914$ (4) Å; I···C(18) $(-x+1, -y+1, -z+1) = 3\cdot968$ (13) Å.

The molecular symmetry approximates to an m plane defined by Cl, C(22), C(19), C(3), N(6) and C(25). The crystal packing is mainly determined by Coulombic and van der Waals forces. The intermolecular non-bonding distances correspond to standard van der Waals values.

References

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press.

JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee.

MARTÍNEZ-RIPOLL, M. & CANO, F. H. (1975). *PESOS*. Instituto Rocasolano, CSIC, Madrid, Spain.

NARDELLI, M. (1982). *PARST*. Instituto di Chimica Generale, Univ. of Parma, Italy.

SMITH-VERDIER, P., FLORENCIO, F. & GARCÍA-BLANCO, S. (1983). 8th Eur. Crystallogr. Meet., 2–12 August 1983, Liège, Belgium, Abstract 2b, 16-P.

STEWART, J. M., KUNDELL, F. A. & BALDWIN, J. C. (1970). The *XRAY*70 system. Computer Science Center, Univ. of Maryland, College Park, Maryland.

Structure of 2-[4-(Acetylaminosulphonyl)phenylcarbamoyl]benzoic Acid (Phthalylsulfacetamide), $C_{16}H_{14}N_2O_6S$

BY T. P. SINGH,* URMILA PATEL AND M. HARIDAS

*Department of Physics, Sardar Patel University, Vallabh Vidyanagar 388 120, India*

Abstract. $M_r = 362\cdot37$, monoclinic, $P2_1/c$, $a =$ 8·01 (2), $b = 13\cdot00$ (2), $c = 18\cdot04$ (3) Å, $\beta =$ 111·6 (5)°, $V = 1747$ (6) Å^3, $Z = 4$, $D_m = 1\cdot386$ (5), $D_x = 1\cdot378$ (5) Mg m^{-3}, $\lambda(Cu\,K\alpha) = 1\cdot5418$ Å, $\mu =$ 1·98 mm^{-1}, $F(000) = 816$, $T = 297$ K, final $R = 0\cdot092$ for 1803 observed reflections. The two planar benzene rings in the structure make an angle of 62·1 (5)° with each other. The molecules are arranged in the form of hydrogen-bonded loops. There are no intermolecular interactions in the interior of the loop. The density of crystals is lower than that observed in other sulphonamides. The molecule adopts a coiled conformation about the a axis.

* To whom correspondence should be addressed. Present address: Department of Biophysics, All India Institute of Medical Sciences, New Delhi-110029, India.

Introduction. The sulphonamides constitute an important class of antimicrobial agents which exert antibacterial action by inhibiting the enzyme dihydropteroate synthase competitively towards the substrate p-aminobenzoate (PAB). This enzyme catalyses the formation of dihydropteroate from PAB and hydroxy-methyldihydropteridine pyrophosphate (Brown, 1971) so that its inhibition leads to bacteriostasis. A detailed study of the structural features of inhibitors in relation to their biological activity is an important step towards the deduction of the interaction mechanisms of enzyme inhibition and provides useful knowledge for the design of the most suitable molecules according to the stereo-electronic requirements of the inhibitory interaction. As part of our programme of systematic X-ray structural studies on sulphonamides and their receptor molecules (Haridas, Tiwari & Singh, 1984), we report here the crystal structure of phthalylsulfacet-amide.
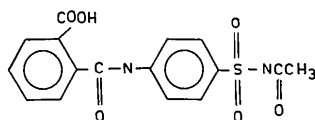
Experimental. Samples of phthalylsulfacetamide obtained from Indian Drugs and Pharmaceuticals Ltd, Hyderabad; rectangular colourless crystals by slow evaporation from a solution in a mixture of acetone and methanol at 297 K. Crystal $1.20 \times 0.50 \times 0.47$ mm. Unit-cell dimensions and space group from oscillation and Weissenberg photographs. Density by flotation in benzene/carbon tetrachloride. Intensity data from multiple-film equi-inclination Weissenberg photographs, estimated visually; Ni-filtered Cu $K\alpha$ radiation; 3763 reflections recorded, 1803 unique reflections observed (h 0–7, k 0–16, l −22–18, $4.9 \leq 2\theta \leq 91.6°$). Corrections for Lorentz and polarization effects and for spot-shape distortions but not for absorption. Layerwise and overall scale factors obtained from Wilson's (1942) statistics. Partial structure by *MULTAN* (Germain, Main & Woolfson, 1971), remaining non-H atoms by subsequent $\Delta\rho$ maps. Non-H atoms refined anisotropically. H-atom positions from $\Delta\rho$ maps but not refined. f values for non-H atoms from Cromer & Waber (1965), and Stewart, Davidson & Simpson (1965) for H atoms. $(\Delta/\sigma)_{ave} = 0.14$, $(\Delta/\sigma)_{max} = 0.23$ for non-H atoms. $R = 0.092$, $wR = 0.096$, $S = 0.53$. 58 strongest low-angle reflections corrected for secondary extinction with empirical extinction correction coefficient $g = 0.0001$ where $F_{corr} = F_o(1 + 2gF_c^2)^{1/2}$ (Stout & Jensen, 1968). Final $\Delta\rho$ excursions -0.26 to 0.29 e Å^{-3}. Weighting function $w = 1/(0.80 + 0.01|F_o| - 0.0015|F_o|^2)$ (Cruickshank, 1961) 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. All calculations on the MS University, Baroda, IBM 360/44 computer.

Table 1. *Fractional coordinates* $(\times 10^4)$ *of the non-hydrogen atoms and equivalent isotropic thermal parameters* $(\times 10^4)$ *with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{1}{3}(B_{11} + B_{22} + B_{33}).$$

	x	y	z	B_{eq}(Å^2)
C(1)	−65 (21)	3750 (11)	3581 (9)	42 (16)
C(2)	588 (23)	3901 (13)	4424 (8)	59 (18)
C(3)	2401 (22)	3832 (13)	4888 (9)	49 (17)
C(4)	3616 (21)	3585 (11)	4516 (8)	39 (15)
C(5)	2938 (25)	3481 (15)	3686 (10)	62 (20)
C(6)	1135 (25)	3583 (15)	3283 (9)	81 (20)
N(7)	5489 (16)	3400 (10)	4936 (7)	27 (12)
S(8)	−2398 (5)	3858 (3)	3001 (2)	27 (3)
O(9)	−2627 (16)	4307 (9)	2242 (6)	62 (13)
O(10)	−3289 (16)	4328 (9)	3466 (7)	65 (13)
N(11)	−3111 (17)	2648 (9)	2773 (7)	35 (13)
C(12)	−3119 (20)	1909 (11)	3335 (8)	37 (15)
O(13)	−2742 (19)	2157 (9)	4030 (6)	102 (16)
C(14)	−3603 (30)	840 (14)	3040 (12)	113 (25)
C(15)	6331 (22)	3110 (11)	5741 (8)	51 (17)
O(16)	5685 (15)	3245 (9)	6233 (6)	58 (12)
C(17)	8224 (19)	2721 (10)	5957 (7)	25 (14)
C(18)	9669 (25)	3360 (13)	6342 (10)	58 (21)
C(19)	11385 (23)	3009 (15)	6528 (11)	41 (18)
C(20)	11748 (21)	2017 (14)	6320 (10)	40 (18)
C(21)	10330 (20)	1355 (13)	5950 (9)	38 (16)
C(22)	8540 (19)	1659 (11)	5769 (8)	34 (15)
C(23)	6997 (20)	945 (11)	5411 (9)	33 (15)
O(24)	7505 (16)	11 (9)	5256 (9)	66 (14)
O(25)	5460 (13)	1171 (8)	5304 (6)	35 (11)

Table 2. *Bond lengths* (Å) *and bond angles* (°) *involving non-hydrogen atoms with e.s.d.'s in parentheses*

C(1)–C(2)	1.43 (2)	C(12)–O(13)	1.22 (2)
C(1)–C(6)	1.34 (3)	C(12)–C(14)	1.49 (2)
C(1)–S(8)	1.78 (1)	C(15)–O(16)	1.19 (2)
C(2)–C(3)	1.39 (2)	C(15)–C(17)	1.51 (2)
C(3)–C(4)	1.41 (3)	C(17)–C(18)	1.39 (2)
C(4)–C(5)	1.40 (2)	C(17)–C(22)	1.47 (2)
C(4)–N(7)	1.43 (2)	C(18)–C(19)	1.37 (3)
C(5)–C(6)	1.38 (2)	C(19)–C(20)	1.40 (3)
N(7)–C(15)	1.41 (2)	C(20)–C(21)	1.39 (2)
S(8)–O(9)	1.44 (1)	C(21)–C(22)	1.40 (2)
S(8)–O(10)	1.42 (1)	C(22)–C(23)	1.49 (2)
S(8)–N(11)	1.67 (1)	C(23)–O(24)	1.34 (2)
N(11)–C(12)	1.40 (2)	C(23)–O(25)	1.21 (2)

C(2)–C(1)–C(6)	118.1 (15)	N(11)–C(12)–C(14)	116.9 (14)
C(2)–C(1)–S(8)	120.6 (12)	O(13)–C(12)–C(14)	123.2 (15)
C(6)–C(1)–S(8)	121.3 (13)	N(7)–C(15)–O(16)	123.6 (14)
C(1)–C(2)–C(3)	121.7 (15)	N(7)–C(15)–C(17)	114.3 (13)
C(2)–C(3)–C(4)	118.8 (15)	O(16)–C(15)–C(17)	121.8 (14)
C(3)–C(4)–C(5)	117.9 (15)	C(15)–C(17)–C(18)	120.2 (14)
C(3)–C(4)–N(7)	124.1 (13)	C(15)–C(17)–C(22)	120.0 (12)
C(5)–C(4)–N(7)	118.0 (14)	C(18)–C(17)–C(22)	119.8 (14)
C(4)–C(5)–C(6)	121.9 (17)	C(17)–C(18)–C(19)	120.1 (16)
C(1)–C(6)–C(5)	121.4 (17)	C(18)–C(19)–C(20)	122.0 (17)
C(4)–N(7)–C(15)	127.0 (12)	C(19)–C(20)–C(21)	119.1 (16)
C(1)–S(8)–O(9)	109.3 (7)	C(20)–C(21)–C(22)	121.5 (15)
C(1)–S(8)–O(10)	109.5 (7)	C(17)–C(22)–C(21)	117.4 (13)
C(1)–S(8)–N(11)	105.1 (7)	C(17)–C(22)–C(23)	120.0 (13)
O(9)–S(8)–N(11)	103.6 (7)	C(21)–C(22)–C(23)	122.6 (14)
O(10)–S(8)–N(11)	110.5 (7)	C(22)–C(23)–O(24)	112.8 (13)
O(9)–S(8)–O(10)	118.1 (7)	C(22)–C(23)–O(25)	123.5 (14)
S(8)–N(11)–C(12)	124.0 (10)	O(24)–C(23)–O(25)	123.7 (14)
N(11)–C(12)–O(13)	119.9 (14)		

Discussion. The final positional parameters of the non-H atoms are given in Table 1.* The interatomic distances and angles are listed in Table 2. The numbering scheme and a perspective view of the molecule are shown in Fig. 1. The average C—H and N—H distances in the molecule are 0·9 and 1·0 Å respectively. The bond lengths and angles in the benzene rings have characteristic values. The C(1)—S(8) distance of 1·78 (1) Å is a normal single-bond value and matches well with those observed in other sulphonamides (Haridas, Tiwari & Singh, 1984). The S(8)—N(11) distance of 1·67 (1) Å is slightly longer than the values found in other sulphonamides (Alléaume, Gulko, Herbstein, Kapon & Marsh, 1976). The S—N bond distance in sulphamic acid (Sass, 1960) is 1·764 (3) Å (by neutron diffraction) and thus S(8)—N(11) in this structure must have a considerable amount of double-bond character. The S(8)—O(9) and S(8)—O(10) distances of 1·44 (1) and 1·42 (1) Å are similar to those found in analogous structures. These distances do not change significantly in the sulphonamide structures (Chatterjee, Dattagupta & Saha, 1981) despite variable intermolecular interactions through them. The angular disposition of the bonds about S(8) deviates significantly from that of a regular tetrahedron with the largest angle O(9)—S(8)—O(10) [118·1 (7)°] and the smallest O(9)—S(8)—N(11) [103·6 (7)°].

The two planar benzene rings in the structure are rotated 62·1 (5)° with respect to each other. The molecule is capable of a variety of conformational states by means of rotations about the bonds C(1)—S(8), S(8)—N(11), N(11)—C(12), C(4)—N(7), N(7)—C(15) and C(15)—C(17). The dihedral angles describing these conformations are C(2)—C(1)—S(8)—N(11) 74·8 (2), C(1)—S(8)—N(11)—C(12) −115·4 (2), S(8)—N(11)—C(12)—C(14)   6·7 (2),   C(3)—C(4)—N(7)—

C(15)   −158·4 (2),   C(14)—N(7)—C(15)—C(17) 14·3 (2) and N(7)—C(15)—C(17)—C(22) 99·9 (2)°.

The molecule adopts a somewhat coiled conformation about the *a* axis. The distance, on the projection plane down the *a* axis, between the terminal atoms O(13) and O(25) is 1·27 Å. The molecular packing of phthalylsulfacetamide as viewed down the *a* axis is shown in Fig. 2. The molecules are arranged in the form of hydrogen-bonded loops. The hydrogen bonds are of the N—H···O and O—H···O types and are indicated in Fig. 2. The imino nitrogen N(11) is bonded to O(16) of the symmetry-related molecule [2·83 (2) Å, 152·8°]. The carboxylic groups of the centrosymmetrically related molecules are involved in a pair of O(24)—H(24)···O(25) hydrogen bonds [2·65 (2) Å, 156·2°]. The molecular stacking along the *a* axis is achieved by a hydrogen bond through N(7) and O(13)[1 + *x, y, z*] [3·00 (2) Å, 166·7°] and some intermolecular van der Waals interactions.

The network of strong hydrogen bonds and van der Waals interactions provides a very compact packing along the hydrogen-bonded loop described above and in the perpendicular direction. However, the interior of the loop is completely devoid of any significant intermolecular interaction [the closest intermolecular distance across the loop is 3·51 (2) Å], *i.e.* there is a considerable unoccupied volume surrounded by the loop. Consequently, in the present structure:

(1) the density [$D_x = 1·378$ (5) Mg m^{-3}] is lower than that found in other sulphonamides (Table 3);

(2) there are a large number of unobserved reflections (recorded 3763, observed 1803);

(3) there is a pronounced secondary-extinction effect;

(4) the temperature factors have low values ($B_{iso} \simeq 2·50$ Å^2).

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond distances, least-squares planes and intermolecular contact distances have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39672 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
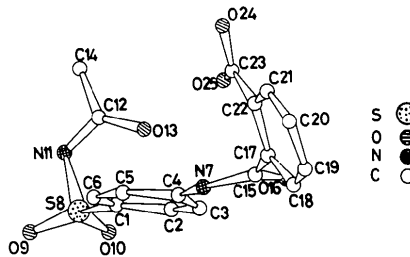

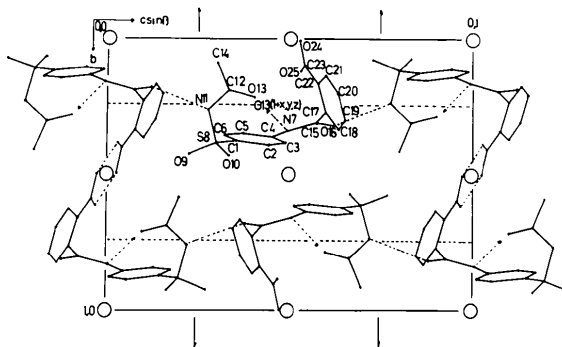Fig. 1. A perspective view of the molecule along the *a* axis and the numbering scheme.

Fig. 2. The crystal structure as seen down the *a* axis. The dotted lines indicate the hydrogen bonds.

Table 3. *Densities of sulphonamide crystals*

Compound	Density (Mg m⁻³)	Reference
Phthalylsulfacetamide	1·378	Present structure
Sulfadimidine	1·423	Tiwari, Haridas & Singh (1984)
Sulfadiazine	1·51	Joshi, Tiwari, Patel & Singh (1983)
Sulfadimethoxine	1·47	Patel, Tiwari, Patel & Singh (1983)
Sulfamethoxazole	1·493	Bettinetti, Giordano, La Manna, Giuseppetti & Tadini (1982)
Sulfamerazine	1·43	Acharya, Kuchela & Kartha (1982)
Sulfisoxazole	1·418	Chatterjee, Dattagupta & Saha (1982)
4 Homosulphanilamide hydrochloride	1·43	Chatterjee, Dattagupta & Saha (1981)
Anhydrous sulfaguanidine	1·563	Kálmán, Czugler & Argay (1981)
Succinylsulfathiazole monohydrate	1·52	Rodier, Chauvet & Masse (1978)
Methanesulphonamide of morpholine (MSM)	1·426	Perales & Garcia-Blanco (1977)
Sulthiame	1·52	Camerman & Camerman (1975)
Sulfathiazole form I	1·499	
form II	1·550	Kruger & Gafner (1972)
form III	1·567	
2'-Hydroxymethanesulphonanilide	1·509	Klug (1970)
Methanesulphonanilide	1·41	Klug (1968)
Sulphanilamide monohydrate	1·495	Alléaume & Decap (1968)
β-Sulphanilamide	1·514	O'Connell & Maslen (1967)
γ Sulphanilamide	1·486	Alléaume & Decap (1965)
α Sulphanilamide	1·479	O'Connor & Maslen (1965)
Sulphanilic acid monohydrate	1·576	Rae & Maslen (1962)

References

ACHARYA, K. R., KUCHELA, K. N. & KARTHA, G. (1982). *J. Cryst. Spectrosc. Res.* **12**, 369–376.

ALLÉAUME, M. & DECAP, J. (1965). *Acta Cryst.* **19**, 934–938.

ALLÉAUME, M. & DECAP, J. (1968). *Acta Cryst.* B**24**, 214–222.

ALLÉAUME, M., GULKO, A., HERBSTEIN, F. H., KAPON, M. & MARSH, R. E. (1976). *Acta Cryst.* B**32**, 669–682.

BETTINETTI, G. P., GIORDANO, F., LA MANNA, A., GIUSEPPETTI, G. & TADINI, C. (1982). *Cryst. Struct. Commun.* **11**, 821–828.

BROWN, G. M. (1971). *Adv. Biochem.* **35**, 35–40.

CAMERMAN, A. & CAMERMAN, N. (1975). *Can. J. Chem.* **53**, 2194–2198.

CHATTERJEE, C., DATTAGUPTA, J. K. & SAHA, N. N. (1981). *Acta Cryst.* B**37**, 1835–1838.

CHATTERJEE, C., DATTAGUPTA, J. K. & SAHA, N. N. (1982). *Acta Cryst.* B**38**, 1845–1847.

CROMER, D. T. & WABER, J. T. (1965). *Acta Cryst.* **18**, 104–109.

CRUICKSHANK, D. W. J. (1961). In *Computing Methods and the Phase Problem in X-ray Crystal Analysis.* Oxford: Pergamon Press.

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

HARIDAS, M., TIWARI, R. K. & SINGH, T. P. (1984). *Acta Cryst.* C**40**, 658–660.

JOSHI, V. V., TIWARI, R. K., PATEL, T. C. & SINGH, T. P. (1983). *Indian J. Phys.* **57A**, 79–89.

KÁLMÁN, A., CZUGLER, M. & ARGAY, GY. (1981). *Acta Cryst.* B**37**, 868–877.

KLUG, H. P. (1968). *Acta Cryst.* B**24**, 792–802.

KLUG, H. P. (1970). *Acta Cryst.* B**26**, 1268–1275.

KRUGER, G. J. & GAFNER, G. (1972). *Acta Cryst.* B**28**, 272–283.

O'CONNELL, A. M. & MASLEN, E. N. (1967). *Acta Cryst.* **22**, 134–145.

O'CONNOR, B. H. & MASLEN, E. N. (1965). *Acta Cryst.* **18**, 363–366.

PATEL, U. TIWARI, R. K., PATEL, T. C. & SINGH, T. P. (1983). *Indian J. Phys.* **57A**, 90–99.

PERALES, A. & GARCÍA-BLANCO, S. (1977). *Acta Cryst.* B**33**, 3169–3172.

RAE, A. I. M. & MASLEN, E. N. (1962). *Acta Cryst.* **15**, 1285–1291.

RODIER, N., CHAUVET, A. & MASSE, J. (1978). *Acta Cryst.* B**34**, 218–221.

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

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

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

STOUT, G. H. & JENSEN, L. H. (1968). *X-ray Structure Determination*, p. 411. London: Collier–Macmillan.

TIWARI, R. K., HARIDAS, M. & SINGH, T. P. (1984). *Acta Cryst.* C**40**, 655–657.

WILSON, A. J. C. (1942). *Nature (London).* **150**, 151–152.

Etude des Composés à Chaînes Aliphatiques.
3. Structure du Bis(*n*-heptanoate) de Pipérazinium, C₄H₁₂N₂²⁺.2C₇H₁₃O₂⁻

PAR JEAN-PIERRE SANGIN ET FRANÇOIS BRISSE

Département de Chimie, Université de Montréal, CP 6210, Succ. A, Montréal, Québec, Canada H3C 3V1

Abstract. $M_r = 346\cdot51$, m.p. 370 K, triclinic, $P\bar{1}$, $a = 5\cdot759$ (2), $b = 7\cdot549$ (2), $c = 12\cdot452$ (2) Å, $\alpha = 95\cdot21$ (5), $\beta = 95\cdot25$ (4), $\gamma = 100\cdot21$ (4)°, $V = 527\cdot3$ Å³, $Z = 1$, $D_m = 1\cdot06$, $D_x = 1\cdot091$ Mg m⁻³, $F(000) = 192$, $\mu(\text{Mo } K\alpha) = 0\cdot71$ mm⁻¹, $\lambda(\text{Mo } K\alpha) = 0\cdot71069$ Å, $T = 293$ K, final $R = 0\cdot044$ for 1144 observed reflections. The structure consists of a piperazinium cation lying on a crystallographic center of symmetry hydrogen-bonded to two *n*-heptanoate anions. These anions have the fully extended conformation while the carboxylate group is tilted by 54° from the plane of the methylenic chain.

Introduction. Il a été récemment rapporté que les densités et les points de fusion dans la série des bis(*n*-alcanoates) de pipérazinium, $2[C_xH_{2x-1}O_2^-].[C_4H_{12}N_2^{2+}]$, variaient de manière régulière avec le nombre *x* d'atomes de carbone de l'anion. Cependant, les points de fusion se trouvent répartis sur deux courbes distinctes dépendant de la parité de *x*. La majorité des sels de cette série ont des mailles tricliniques, mais il était surprenant de remarquer que si les dimensions *a* et *b* des mailles cristallines ne variaient pratiquement pas avec *x*, par contre la dimension *c* de ces mailles croissait linéairement avec *x*