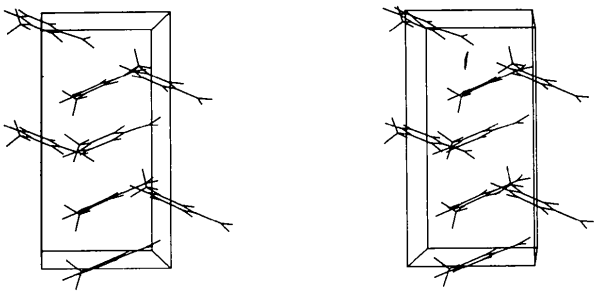

Fig. 2. Vue stéréoscopique suivant l'axe *b* de la structure.

Références

DECLERCQ, J.-P., SCHANCK, A., GERMAIN, G., DEREPPE, J. M. & VAN MEERSSCHE, M. (1977). *Acta Cryst.* B**33**, 3876–3877.

DEREPPE, J. M., SCHANCK, A., DECLERCQ, J.-P., GERMAIN, G. & VAN MEERSSCHE, M. (1976). *Bull. Soc. Chim. Belg.* **85**, 729–733.

DUPONT, L., DIDEBERG, O. & THUNUS, L. (1983). *Acta Cryst.* C**39**, 1407–1410.

GELBCKE, M., GRIMEE, R., LEJEUNE, R., THUNUS, L. & DEJARDIN, J. V. (1983). *Bull. Soc. Chim. Belg.* **92**, 459–463.

GERMAIN, G., DECLERCQ, J.-P., SCHANCK, A., DEREPPE, J. M. & VAN MEERSSCHE, M. (1977). *Acta Cryst.* B**33**, 3878–3880.

International Tables for X-ray Crystallography (1962). Tome III. Birmingham: Kynoch Press.

LEJEUNE, R., VANDENBALCK, J. L., PATRIARCHE, G. J. & LAPIÈRE, C. L. (1981*a*). *Bull. Soc. Chim. Belg.* **90**, 663–674.

LEJEUNE, R., VANDENBALCK, J. L., PATRIARCHE, G. J. & LAPIÈRE, C. L. (1981*b*). *Anal. Lett.* **14**(B15), 1279–1295.

LEJEUNE, R., VANDENBALCK, J. L., PATRIARCHE, G. J. & LAPIÈRE, C. L. (1981*c*). *Anal. Lett.* **14**(A16), 1311–1325.

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. de York, Angleterre, et de Louvain-la-Neuve, Belgique.

NORTH, A. C. T., PHILLIPS, D. C. & MATHEWS, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

SHELDRICK, G. M. (1976). *SHELX*76. Programme pour la détermination de structures cristallines. Univ. de Cambridge, Angleterre.

THUNUS, L. (1981). *J. Pharm. Belg.* **36**, 237–242.

THUNUS, L. & LAPIÈRE, C. L. (1982). *Ann. Pharm. Fr.* **40**, 259–267.

Acta Cryst. (1984). C**40**, 419–422

Structure of Sulphaproxyline (*p*-Isopropoxy-*N*-sulphanilylbenzamide), $C_{16}H_{18}N_2O_4S$

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Abstract. $M_r = 334{\cdot}40$, monoclinic, $P2_1/c$, $a = 9{\cdot}908$ (2), $b = 17{\cdot}263$ (2), $c = 9{\cdot}585$ (1) Å, $\beta = 103{\cdot}08$ (2)°, $V = 1596{\cdot}9$ (4) Å^3, $Z = 4$, $D_m = 1{\cdot}393$, $D_x = 1{\cdot}391$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å, $\mu = 0{\cdot}266$ mm^{-1}, $F(000) = 704$, $T = 296$ K, final $R = 0{\cdot}043$ using 1983 observed reflections. The structure is compared with that of similar sulphonamides, particularly with sulphacetamide and its 1:1 complex with caffeine. In packing, the molecules are extended along the *b* axis. Of the three available H atoms, only the amido H forms an intermolecular hydrogen bond with a keto O forming an infinite chain in the direction of the *c* axis.

Introduction. Sulphaproxyline, SPX (Fig. 1), belongs to the sulphonamide group of drugs which are known to have antibacterial activity. It is generally used in 1:1 ratio with another sulphonamide, sulphamerazine, which exerts a synergic antibacterial effect. The advantage of this combination is that the two active constituents as well as their metabolites are readily soluble in acid urine preventing the formation of crystalluria even at strong acidic pH.

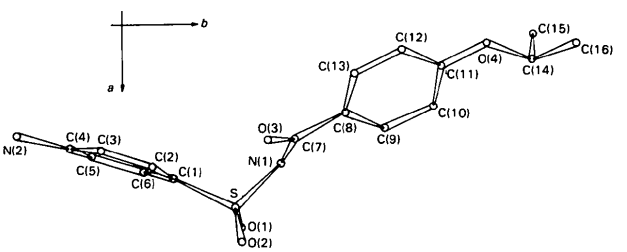

Fig. 1. View of the molecule down the *c* axis.

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The structural study of this *N*-substituted sulphonamide was undertaken in continuation of our studies on substituted sulphonamides reported earlier (Basak, Mazumdar & Chaudhuri, 1982, 1983). Moreover, this study offered us an opportunity to determine the conformational changes in this molecule with respect to sulphacetamide (Basak *et al.*, 1982), with the methyl group in the latter replaced by a *p*-substituted phenyl ring.

Experimental. Transparent monoclinic crystals (from acetone), density by flotation (KI solution). Symmetry from X-ray photographs ($P2_1/c$; $0k0$ absent for k odd, $h0l$ absent for l odd). Crystal $0.32 \times 0.17 \times 0.15$ mm. Enraf-Nonius CAD-4 diffractometer, graphite-monochromatized Mo $K\alpha$. Accurate cell parameters from 25 high-angle reflections, $16° \le \theta \le 19°$. 2802 unique reflections ($-11 \le h \le 11$, $0 \le k \le 20$, $0 \le l \le 11$; $2° \le \theta \le 25°$), 1983 'observed' with $I \ge 3\sigma(I)$. Lp correction, absorption ignored. Correction for intensity variation (<2%). Direct methods (*MULTAN*78, Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). Anisotropic full-matrix refinement based on F (*ORFLS*, Busing, Martin & Levy, 1962); H (from ΔF synthesis) isotropic. $R = 0.043$, $R_w = 0.053$, $S = 1.819$, $w = 1/\sigma^2(|F_o|)$. $(\Delta/\sigma)_{max} < 0.01$. Peak heights -0.25 to 0.23 e Å^{-3} in final ΔF synthesis. Scattering factors for non-H atoms from Cromer & Waber (1965), for H from Stewart, Davidson & Simpson (1965). Anomalous-dispersion corrections for all non-H atoms from *International Tables for X-ray Crystallography* (1974).

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters (Hamilton, 1959) with e.s.d.'s in parentheses*

$B_{eq} = \frac{8}{3}\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}(Å^2)
S	0·49006 (8)	0·16330 (4)	0·74238 (7)	3·00
O(1)	0·5432 (2)	0·1719 (1)	0·6160 (2)	3·98
O(2)	0·5822 (2)	0·1734 (1)	0·8797 (2)	4·01
O(3)	0·3097 (2)	0·2139 (1)	0·9360 (2)	3·17
O(4)	0·0557 (2)	0·5479 (1)	0·8023 (2)	4·08
N(1)	0·3719 (2)	0·2323 (1)	0·7250 (2)	2·97
N(2)	0·2951 (3)	−0·1584 (2)	0·7456 (3)	5·69
C(1)	0·4099 (3)	0·0733 (2)	0·7372 (3)	2·99
C(2)	0·3795 (4)	0·0413 (2)	0·8598 (3)	4·28
C(3)	0·3376 (4)	−0·0346 (2)	0·8589 (3)	4·65
C(4)	0·3275 (3)	−0·0810 (2)	0·7391 (3)	3·60
C(5)	0·3504 (3)	−0·0469 (2)	0·6161 (3)	4·01
C(6)	0·3915 (3)	0·0289 (2)	0·6140 (3)	3·45
C(7)	0·3076 (3)	0·2556 (1)	0·8319 (2)	2·57
C(8)	0·2402 (3)	0·3321 (1)	0·8126 (2)	2·48
C(9)	0·2836 (3)	0·3914 (1)	0·7350 (3)	2·75
C(10)	0·2249 (3)	0·4642 (2)	0·7283 (3)	3·09
C(11)	0·1192 (3)	0·4786 (2)	0·7977 (3)	3·00
C(12)	0·0734 (3)	0·4192 (2)	0·8737 (3)	3·53
C(13)	0·1336 (3)	0·3475 (2)	0·8820 (3)	3·21
C(14)	0·1012 (3)	0·6157 (2)	0·7368 (3)	3·62
C(15)	0·0336 (4)	0·6185 (2)	0·5795 (4)	6·20
C(16)	0·0604 (4)	0·6829 (2)	0·8195 (4)	4·82

Discussion. The final atomic coordinates for the non-hydrogen atoms together with their temperature factors are listed in Table 1.* The intramolecular bond distances and angles and some selected torsion angles are listed in Table 2.

The S atom exhibits the usual distorted tetrahedral configuration with bond lengths and angles involving it lying within the ranges quoted in the literature (Alléaume, Gulko, Herbstein, Kapon & Marsh, 1976). The intramolecular contacts O(1)—O(2) [2·469 (3) Å], O(1)—N(1) [2·421 (3) Å] and O(2)—N(1) [2·485 (3) Å] are comparable with the values observed in the crystal structures of dibenzenesulphonamide and its sodium salt (Cotton & Stokley, 1970), sulphacetamide {*N*-[(4-aminophenyl)sulphonyl]acetamide} (Basak *et al.*, 1982) and sulphamethazine [4-amino-*N*-(4,6-dimethyl-2-pyrimidinyl)benzenesulphonamide] (Basak *et al.*, 1983).

The S—N(1) and S—C(1) bond distances are shorter than the corresponding single-bond distances; this shortening has been attributed to $d\pi$—$p\pi$ interactions

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, least-squares-planes' data and torsion angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38951 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond distances* (Å), *bond angles* (°) *and selected torsion angles* (°)

S—O(1)	1·434 (2)	S—O(2)	1·432 (2)
S—N(1)	1·652 (2)	S—C(1)	1·741 (3)
N(1)—C(7)	1·383 (3)	C(7)—O(3)	1·227 (3)
C(7)—C(8)	1·472 (3)	C(8)—C(9)	1·390 (3)
C(9)—C(10)	1·380 (4)	C(10)—C(11)	1·384 (4)
C(11)—C(12)	1·392 (4)	C(12)—C(13)	1·368 (5)
C(13)—C(8)	1·395 (4)	C(1)—C(2)	1·392 (4)
C(2)—C(3)	1·374 (5)	C(3)—C(4)	1·385 (4)
C(4)—C(5)	1·382 (4)	C(5)—C(6)	1·372 (5)
C(6)—C(1)	1·385 (4)	C(4)—N(2)	1·379 (5)
C(11)—O(4)	1·357 (4)	O(4)—C(14)	1·448 (4)
C(14)—C(15)	1·506 (5)	C(14)—C(16)	1·511 (5)
O(1)—S—O(2)	119·0 (1)	C(11)—O(4)—C(14)	120·4 (2)
O(1)—S—N(1)	103·1 (1)	S—N(1)—C(7)	124·7 (2)
O(1)—S—C(1)	108·7 (1)	S—C(1)—C(2)	121·0 (2)
O(2)—S—N(1)	107·1 (1)	S—C(1)—C(6)	119·3 (2)
O(2)—S—C(1)	109·1 (1)	N(2)—C(4)—C(3)	119·8 (3)
N(1)—S—C(1)	109·4 (1)	N(2)—C(4)—C(5)	122·4 (3)
C(2)—C(1)—C(6)	119·2 (3)	O(3)—C(7)—N(1)	120·4 (2)
C(1)—C(2)—C(3)	119·7 (3)	O(3)—C(7)—C(8)	123·5 (2)
C(2)—C(3)—C(4)	121·4 (3)	N(1)—C(7)—C(8)	116·1 (2)
C(3)—C(4)—C(5)	117·8 (3)	C(7)—C(8)—C(9)	122·8 (2)
C(4)—C(5)—C(6)	121·7 (3)	C(7)—C(8)—C(13)	118·8 (2)
C(5)—C(6)—C(1)	119·8 (3)	C(9)—C(8)—C(13)	118·3 (2)
O(4)—C(11)—C(12)	115·1 (3)	C(8)—C(9)—C(10)	121·2 (2)
O(4)—C(11)—C(10)	125·5 (3)	C(9)—C(10)—C(11)	119·8 (3)
O(4)—C(14)—C(15)	110·4 (3)	C(10)—C(11)—C(12)	119·4 (3)
O(4)—C(14)—C(16)	104·3 (2)	C(11)—C(12)—C(13)	120·5 (3)
C(15)—C(14)—C(16)	112·9 (3)	C(8)—C(13)—C(12)	120·8 (3)
C(2)—C(1)—S—N(1)	−84·1 (3)	C(1)—S—N(1)—C(7)	75·6 (2)
C(6)—C(1)—S—N(1)	103·8 (3)	O(1)—S—N(1)—C(7)	−168·8 (2)
C(2)—C(1)—S—O(1)	164·0 (3)	O(2)—S—N(1)—C(7)	−42·5 (2)
C(2)—C(1)—S—O(2)	32·8 (3)	S—N(1)—C(7)—O(3)	−17·9 (3)
C(6)—C(1)—S—O(1)	−8·1 (3)	S—N(1)—C(7)—C(8)	161·4 (2)
C(6)—C(1)—S—O(2)	−139·3 (2)		

between the atoms (Cotton & Stokley, 1970). The C(4)–N(2) and C(7)–N(1) bond lengths are intermediate between the bond orders 1 and 1·5 for the C(sp^2)–N(sp^2) bond (Burke-Laing & Laing, 1976), indicating some π conjugation between N(2) and the arylamino phenyl ring, and between N(1) and the S atom. The enlargement of the S–N(1)–C(7) angle from the normal value of 120° is as found in a number of substituted sulphonamides: 124·8 (2)° in sulphacetamide (Basak *et al.*, 1982), 125·9° in sulphadimethoxine and 126·7° in sulphadoxine (Shefter, Chmielewicz, Blount, Brennan, Sackman & Sackman, 1972). This enlargement of the angle can be attributed to a non-bonded contact [2·984 (2) Å] between the S and the keto O atom, O(3).

In the present structure, the deviations of the constituent atoms from the mean planes of the respective phenyl rings lie within the range +0·019 (4) to −0·030 (3) Å. The distortions in the endocyclic bond angles observed in both rings can be attributed to perturbations in the π-electron systems by substituents (Domenicano, Vaciago & Coulson, 1975). The dihedral angle between the least-squares planes of the two phenyl rings is 51·9 (1)°.

The C(11)–O(4) bond length indicates some degree of conjugation between the isopropoxy group and the phenyl ring (Domiano, Nardelli, Balsamo, Macchia & Macchia, 1979) resulting in coplanarity of the phenyl ring and the C(11)–O(4)–C(14) group. The dissymmetry in the angles at C(11) may be explained as due to the non-bonded contact [2·437 (4) Å] between C(10) and O(14). The C(14)–C(15) and C(14)–C(16) bonds are close to the normal C(sp^3)–C(sp^3) distance.

The SPX molecule is, in principle, capable of assuming a variety of conformational states by means of rotation about the S–N(1), C(1)–S and N(1)–C(7) bonds. The torsion angles C(2)–C(1)–S–N(1) and C(6)–C(1)–S–N(1) lie within the range $|\varepsilon_1| = 70$–120° and C(1)–S–N(1)–C(7) lies within the range $|\varepsilon_2| = 60$–90° (Kálmán, Czugler & Argay, 1981). The S–N(1)–C(7)–C(8) torsion angle of 161·4 (2)° indicates that C(8) is (+)-antiperiplanar to S as in sulphacetamide (Basak *et al.*, 1982) and its 1:1 complex with caffeine (Leger, Alberola & Carpy, 1977). In the present structure, and in the two structures mentioned above, the torsion angles about the C(1)–S, S–N(1) and N(1)–C(7) bonds vary in the ranges 38, 20 and 15°, respectively. These variations may be attributed to the different environments in which the molecules have been studied and, in the case of the present compound, to the bulky substituent at the C(7) position. We can also conclude from the ranges of variation observed that there is more torsional flexibility about the C(1)–S than the S–N(amido) and N(1)–C(7) bonds.

Fig. 2 is a view of the crystal structure projected on to the *bc* plane. The amido nitrogen, N(1), is hydrogen bonded to the keto O atom, O(3), of a glide-related

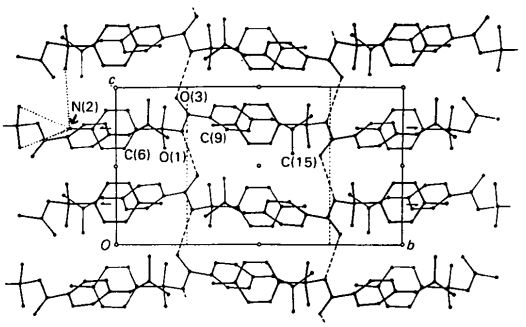

Fig. 2. Projection of the crystal structure on the *bc* plane. The three contacts N(2)···O(1)($1-x$, $-\frac{1}{2}+y$, $\frac{3}{2}-z$), N(2)···O(2)($1-x$, $-\frac{1}{2}+y$, $\frac{3}{2}-z$) and N(2)···O(2)($1-x$, $-y$, $2-z$) are shown by dotted lines.

molecule [N(1)···O(3^i) = 2·853 (3), N(1)–H(N1) = 0·78 (3), H(N1)···O(3^i) = 2·08 (3) Å, ∠N(1)–H(N1)···O(3^i) = 174 (3)°; (i) x, $\frac{1}{2}-y$, $\frac{1}{2}+z$]. The arylamino N atom, N(2), which is the other potential hydrogen-bond donor present in the molecule, does not participate in hydrogen bonding; instead, it is approximately equidistant from three symmetry-related potential hydrogen-bond acceptors [N(2)···O(1)($1-x$, $-\frac{1}{2}+y$, $\frac{3}{2}-z$) = 3·456 (4), N(2)···O(2)($1-x$, $-y$, $2-z$) = 3·531 (3) and N(2)···O(2)($1-x$, $-\frac{1}{2}+y$, $\frac{3}{2}-z$) = 3·466 (4) Å].

The N(1)–H(N1)···O(3^i) hydrogen bonds run in the direction of the *c* axis, effectively forming an infinite chain.

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References

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

BASAK, A. K., MAZUMDAR, S. K. & CHAUDHURI, S. (1982). *Cryst. Struct. Commun.* **11**, 1609–1616.

BASAK, A. K., MAZUMDAR, S. K. & CHAUDHURI, S. (1983). *Acta Cryst.* C**39**, 492–494.

BURKE-LAING, M. & LAING, M. (1976). *Acta Cryst.* B**32**, 3216–3224.

BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1962). *ORFLS*. Report ORNL-TM-306. Oak Ridge National Laboratory, Tennessee.

COTTON, F. A. & STOKLEY, P. F. (1970). *J. Am. Chem. Soc.* **92**, 294–302.

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

DOMENICANO, A., VACIAGO, A. & COULSON, C. A. (1975). *Acta Cryst.* B**31**, 221–234.

DOMIANO, P., NARDELLI, M., BALSAMO, A., MACCHIA, B. & MACCHIA, F. (1979). *Acta Cryst.* B**35**, 1363–1372.

HAMILTON, W. C. (1959). *Acta Cryst.* **12**, 609–610.

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

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

LEGER, J. M., ALBEROLA, S. & CARPY, A. (1977). *Acta Cryst.* B**33**, 1455–1459.

MAIN, P., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1978). *MULTAN78. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

SHEFTER, E., CHMIELEWICZ, Z. F., BLOUNT, J. F., BRENNAN, T. E., SACKMAN, B. F. & SACKMAN, P. (1972). *J. Pharm. Sci.* **61**, 872–877.

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

Acta Cryst. (1984). C**40**, 422–426

Structures of 5-[3-(4-Carbamoyl-4-piperidinopiperidino)propyl]-3-chloro-10,11-dihydro-5*H*-dibenz[*b*,*f*]azepine (*A*),* $C_{28}H_{37}ClN_4O$, 3-Chloro-5-[3-(2-oxo-1,2,3,5,6,7,8,8a-octahydroimidazo[1,2-*a*]pyridine-3-spiro-4′-piperidino)propyl]-10,11-dihydro-5*H*-dibenz[*b*,*f*]azepine (*B*), $C_{28}H_{35}ClN_4O$, and 5-[3-(2-Oxo-1,2,3,5,6,7,8,8a-octahydroimidazo[1,2-*a*]pyridine-3-spiro-4′-piperidino)propyl]-10,11-dihydro-5*H*-dibenz-[*b*,*f*]azepine (*C*), $C_{28}H_{36}N_4O$

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Abstract. (*A*): $M_r = 481{\cdot}09$, monoclinic, $C2/c$, $a = 27{\cdot}81$ (1), $b = 8{\cdot}589$ (2), $c = 22{\cdot}14$ (1) Å, $\beta = 102{\cdot}82$ (4)°, $U = 5164$ (4) Å^3, $Z = 8$, $D_m = 1{\cdot}23$, $D_x = 1{\cdot}24$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}179$ mm^{-1}, $T = 298$ K, $F(000) = 2064$, $R = 0{\cdot}0639$ for 2566 observed reflexions. (*B*): $M_r = 479{\cdot}07$, triclinic, $P\bar{1}$, $a = 11{\cdot}515$ (5), $b = 11{\cdot}837$ (5), $c = 10{\cdot}744$ (3) Å, $\alpha = 92{\cdot}71$ (3), $\beta = 112{\cdot}73$ (3), $\gamma = 68{\cdot}76$ (3)°, $U = 1255$ (1) Å^3, $Z = 2$, $D_m = 1{\cdot}26$, $D_x = 1{\cdot}28$ Mg m^{-3}, μ(Mo $K\alpha$) $= 0{\cdot}184$ mm^{-1}, $T = 298$ K, $F(000) = 512$, $R = 0{\cdot}0658$ for 3114 observed reflexions. (*C*): $M_r = 444{\cdot}63$, monoclinic, $A2/a$, $a = 27{\cdot}29$ (1), $b = 10{\cdot}254$ (5), $c = 18{\cdot}108$ (5) Å, $\beta = 97{\cdot}20$ (2)°, $U = 5027$ (3) Å^3, $Z = 8$, $D_m = 1{\cdot}17$, $D_x = 1{\cdot}18$ Mg m^{-3}, μ(Mo $K\alpha$) $= 0{\cdot}078$ mm^{-1}, $T = 298$ K, $F(000) = 1920$, $R = 0{\cdot}0620$ for 2851 observed reflexions. These three antischizophrenia drugs each form dimers by paired intermolecular O···H(N) hydrogen bonds at the carbamoyl moieties. The ethylene radical in the dibenzazepine ring is in plane with one benzene ring and is out of plane for the other. The Cl atom of the first compound is connected to the out-of-plane benzene ring at the position *meta* to the N atom. That of the second compound is connected to the in-plane benzene ring at the same position.

Introduction. Compounds (*A*), (*B*) and (*C*) are very similar as shown in Fig. 1. However, the pharmacological spectra and activities for antischizophrenia are remarkably different. The X-ray analyses were carried out to study these pharmacological differences from the viewpoint of the molecular conformations.

Experimental. Experimental data are shown in Table 1. Density measured by flotation in KI solution. Colorless crystals of these compounds ground manually to spheres of diameters of about 0·5 mm. Rigaku AFC-5 four-circle automated diffractometer with graphite-monochromatized Mo $K\alpha$ radiation. Cell dimensions derived from least-squares treatment of the setting angles for 20 reflexions. ω–2θ scan technique, scan rate 8° min^{-1} for ω. Three standard reflexions measured every 100 reflexions: no significant variations in

Table 1. *Experimental data*

Compound	(*A*)	(*B*)	(*C*)
Maximum 2θ (°)	45	50	50
Range of h,k,l	$\pm h,k,l$	$h,\pm k,\pm l$	$h,k,\pm l$
Standard reflections	$\bar{2}04$, 020, $\bar{6}02$	$11\bar{2}$, 111, 121	220, 022, $20\bar{4}$
Intensities measured	3248 [$F > \sigma(F)$]	3636 (all)	3630 [$F > \sigma(F)$]
Unique intensities	2847 [$F > \sigma(F)$]	3546 (all)	3328 [$F > \sigma(F)$]
Intensities $>2{\cdot}5\sigma(F)$	2566	3114	2851
R	0·0639	0·0658	0·0620
wR ($w = 1{\cdot}0$)	0·0586	0·0747	0·0623
S	3·12	1·18	2·57
Residual density (e Å^{-3})	<0·95	<0·62	<0·22
$(\Delta/\sigma)_{max}$ for non-H atoms	0·87	0·25 (except disordered parts)	0·67

* IUPAC name: 1′-[3-(3-chloro-10,11-dihydro-5*H*-dibenz[*b*,*f*]-azepin-5-yl)propyl][1,4′-bipiperidine]-4′-carboxamide.

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