In both structures, the hordenine molecules are hydrogen bonded in a head-to-tail fashion (Fig. 2), with N···O 2·75 (1) Å in the orthorhombic form and 2·69 (1) Å in the monoclinic form, giving rise to four or two chains of molecules per unit cell, running parallel to the *a* and *b* axes, respectively.

The position of H(O) is critical as its attachment determines whether the molecule is zwitterionic or neutral. As the atom was located and successfully refined in both structures, the molecule is shown to be non-ionic. This is in agreement with acid ionization constants in aqueous solution which show the *p*-OH to be less acidic than a protonated amino group.

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Platelet Activating Factor Antagonists. Structure of *N,N'*-Bis(3,4,5-trimethoxybenzoyl)-2-piperazinylmethyl 2,2-Dimethylpropanoate

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(*Received* 21 *September* 1990; *accepted* 2 *November* 1990)

Abstract. Racemic title compound, $C_{30}H_{40}N_2O_{10}$, M_r = 588·65, triclinic, $P\bar{1}$, a = 10·154 (7), b = 11·820 (9), c = 15·038 (8) Å, α = 96·02 (5), β = 107·54 (4), γ = 110·34 (5)°, V = 1569 (2) Å^3, Z = 2, D_x = 1·25 g cm^{-3}, Cu $K\alpha$, λ = 1·5418 Å, μ = 7·4 cm^{-1}, $F(000)$ = 628, T = 293 K, R = 0·0470, wR = 0·0481 for 1961 unique observed reflections. The piperazine ring adopts a chair conformation and the molecule shows limited flexibility of the pseudo-twofold-related trimethoxybenzoyl moieties. The planes through the piperazine and the two trimethoxyphenyl rings are oriented almost perpendicular to each other. Apart from a few possible weak hydrogen bonds, the molecules are held together by weak π overlap and van der Waals forces.

Introduction. Platelet activating factor (PAF, PAF-acether) is an autacoid mediator implicated in a diverse range of pathological conditions including inflammation, various types of vascular disorders and shock (Godfroid & Braquet, 1986; Braquet & Godfroid, 1987; Braquet, Touqui, Shen & Vargaftig, 1987). Since the first development of PAF antagonists in 1983 a broad variety of naturally and synthetically derived compounds have been increasingly studied for their remarkable and different biological PAF activities. The characterization of the high-affinity PAF receptor site and molecular design of PAF antagonists are of prime interest for therapeutical purposes in the development of new and efficacious pharmaceutical agents. Recently (Dive, Godfroid, Lamotte-Brasseur, Batt, Heymans, Dupont & Braquet, 1989; Godfroid, Dive, Lamotte-Brasseur & Heymans, 1990), the conformational and electronic properties of some heterogeneous but potent antagonists have been studied in order to find the major and common features that may be of relevance for the control of biological activity. These

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0108-2701/91/071453-05$03.00

results have led to the suggestion of a simplified receptor model called the *cache-oreilles* (ear-muff) model, where two positively charged areas correspond to negative wells of electrostatic potential around the antagonistic molecule at a distance of 12–14 Å and an angle of 180° from each other.

Crystal structures from different categories of PAF antagonists have been reported. Analyses of the conformationally rigid ginkgolides, with the parent compound BN52021* (Dupont, Dideberg, Germain & Braquet, 1986) and the two closely related derivatives, BN52020† and BN52022‡ (Sbit, Dupont, Dideberg & Braquet, 1987), have shown that small molecular changes in the substituents (*e.g.* substituting OH for H) have pronounced effects on the biological activity without considerable changes to the overall solid-state conformation. Recently, the X-ray structures of three semi-rigid furanoid congeners have been reported (Peterson, Smillie & Rogers, 1989; Peterson, Do & Rogers, 1989; Peterson, Horsley, Brozik & Rogers, 1989). These crystal structures have been elucidated not only to provide detailed information about the conformations of the molecules but also to improve the knowledge of the required structural features at the PAF acceptor site through an intimate study of the intermolecular interactions in the crystals. The structurally flexible WEB2086,§ belonging to the triazolothienodiazepine compounds, is one of the most potent PAF antagonists known so far. The WEB compounds are closely related to the famous benzodiazepine family which was first recognized for its psychotropic activity. The X-ray structure of brotizolam,¶ the 2-bromo analogue of WEB2086 with extremely high affinity for the benzodiazepine receptor, has been published (Butcher & Hamor, 1985).

As a consequence of the *cahe-oreilles* model we have since synthesized new and highly potent piperazine analogues possessing the required electronic properties to fit the receptor. In order to provide better information about their stable conformations we shall describe here the X-ray crystal structure of *N*,*N*′-bis(3,4,5-trimethoxybenzoyl)-2-piperazinylmethyl 2,2-dimethylpropanoate (Godfroid, Heymans, Dive, Pirotsky & Braquet, 1989).

Experimental. Colourless prismatic crystals of the title compound were obtained by slow evaporation from dimethyl chloride:ether 1:1 at room temperature. All X-ray measurements were made on a Stoe four-circle diffractometer with monochromatic Cu $K\alpha$ radiation, using a crystal of dimensions 0·32 × 0·40 × 0·12 mm. Accurate unit-cell constants were determined by a least-squares fit of 2θ values for 20 reflections in the θ range 35–48°. The intensity data were collected to a maximum 2θ of 136° by the ω–2θ scan technique. A total of 4487 reflections were measured; 49 steps, $\Delta\omega = 0{\cdot}03°$, 4 steps for background before and after each scan. Min. and max. time per step 0·5 and 2·0 s for prescanned $I/\sigma(I)$ ratios 20·0 and 3·0. The $\sigma(I)$ values were derived from counting statistics. Covered range in indices $0 < h < 12$, $-14 < k < 14$, $-18 < l < 18$. The intensities of three standard reflections recorded every 120 min showed no significant variation throughout the data collection. Most reflections at higher 2θ values were weak. The reflection intensities were corrected for geometrical factors and linear decay with the *REDU*4 program (Stoe & Co., 1985). 1961 reflections with $I \geq 2{\cdot}5\sigma(I)$ were considered observed and were used in the subsequent refinement procedures. No correction for absorption was applied.

The structure was solved by direct methods (*MULTAN*80; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). The initial E map, from the solution with the best figure of merit, showed 34 of the 42 non-H atoms. The remaining atoms were located in a subsequent difference map. Refinement based on $\sum w(|F_o| - |F_c|)^2$ by varied two-block full-matrix least squares (121/1961 and 295/1961) was then carried out with anisotropic thermal factors for all non-H atoms except for the methyl carbon atom C(50). This C atom is doubly disordered C(50)/C(50′) and was isotropically refined to take the occupancy 63/37%. The ideal positions of all H atoms were calculated on the basis of stereochemical considerations after a check on an intermediate difference electron density map. The H atoms were placed 1·08 Å from their parent atoms. Four different isotropic group thermal factors were applied for phenyl-H, methyl-H, tertiary-H and general-H atoms. The weighting scheme used in the final refinement was $w^{-1} = \sigma^2(F_o) + 0{\cdot}0002(F_o)^2$. The final R and wR were 4·70 and 4·81%. $S = 1{\cdot}31$. Max. and average shift/e.s.d. parameters in the final cycles of refinement were 0·89 and 0·02, respectively, and the largest negative and positive peaks in the difference electron density calculation were $-1{\cdot}3$ and 1·1 e Å^{-3}. Atomic scattering factors in the analytical

* BN52021, 3-(1,1-dimethylethyl)hexahydro-4,7b,11-trihydroxy-8-methyl-9*H*-1,7a-(epoxymethano)-1*H*,6a*H*-cyclopenta[*c*]furo-[2,3-*b*]furo[3′,2′:3,4]cyclopenta[1,2-*d*]furan-5,9,12(4*H*)-trione monohydrate.

† BN52020, 3-(1,1-dimethylethyl)hexahydro-4,7b-dihydroxy-8-methyl-9*H*-1,7a-(epoxymethano)-1*H*,6a*H*-cyclopenta[*c*]furo[2,3-*b*]-furo[3′,2′:3,4]cyclopenta[1,2-*d*]furan-5,9,12(4*H*)-trione monohydrate.

‡ BN52022, 3-(1,1-dimethylethyl)hexahydro-2,4,7b,11-tetrahydroxy-8-methyl-9*H*-1,7a-(epoxymethano)-1*H*,6a*H*-cyclopenta[*c*]-furo[2,3-*b*]furo[3′,2′:3,4]cyclopenta[1,2-*d*]furan-5,9,12(4*H*)-trione–ethanol 1·5 hydrate.

§ WEB2086, 4-(2-chlorophenyl)-9-methyl-2-(morpholinopropionyl)-6*H*-thieno[3,2-*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepine.

¶ Brotizolam, 2-bromo-4-(2-chlorophenyl)-9-methyl-6*H*-thieno-[3,2-*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepine.

form and anomalous-dispersion factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). All refinements were performed with the *SHELX*76 crystallographic program package (Sheldrick, 1976). The molecular illustrations were generated with *PLUTO* (Motherwell & Clegg, 1978).

Discussion. *Molecular geometry.* A perspective view of the molecule with the adopted atom-numbering scheme is shown in Fig. 1. Final fractional coordinates for non-H atoms with equivalent isotropic thermal parameters are given in Table 1.* From Table 1 it is evident that the C atoms of the *tert*-butyl group as well as some of the methoxy C atoms have anomalously high temperature-factor values, probably as a consequence of disorder. Only the methoxy C atom C(50) was refined with an occupancy of 63%. Bond lengths and bond angles and some selected torsion angles are listed in Table 2. The corresponding average standard deviations are 0·009 Å, 0·6 and 0·8°, respectively. In Fig. 2 the molecule is viewed perpendicular to the piperazine plane, clearly visualizing the highly symmetric molecular configuration. In the following discussion, bond length and angle values will be individually given for the two pseudo-twofold-related trimethoxybenzoyl moieties and labelled after the respective N atoms N(1) and N(4), with the latter value in square brackets.

The piperazine ring adopts a chair conformation. This type of conformation is the most common low-energy form and is often found in molecules with centres of inversion. In the compound studied the strain caused by the *tert*-butylcarboxymethyl side chain is very low and does not seriously influence the almost perfect twofold symmetry adopted by the rest of the molecule. The pseudo-twofold axis passes through the midpoint of the piperazine ring and parallel to the non-bonded C atoms C(2)–C(6) and C(3)–C(5). All bond distances and bond angles of the piperazine framework are within the range of values found in a number of other chair-form piperazines (Rérat, 1960; Koshino, Sasaki & Haisa, 1973; Olansky & Moncrief, 1973; Ko & Moncrief, 1975; Mouillé, Cotrait, Hospital & Marsau, 1975; Lepore, Ganis, Bombieri, Gilli & Montaudo, 1977; Sakurai, Nakamaru, Tsuboyama & Tsuboyama, 1977; Hiramatsu, Sakurai, Tsuboyama & Tsuboyama, 1978; Okamoto, Sekido, Itoh, Noguchi & Hirokawa, 1979; Van Meerssche, Germain, Declercq & Colens, 1979). In this study the angles at the piperazine C atoms are approximately tetrahedral and the

Table 1. *Fractional atomic coordinates for non-H atoms and equivalent isotropic thermal parameters* U_{eq} (Å^2); *e.s.d.'s are given in parentheses*

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
N(1)	0·7778 (4)	0·2903 (3)	0·9356 (3)	0·044 (2)
C(2)	0·8882 (5)	0·2476 (4)	0·9178 (3)	0·044 (2)
C(3)	1·0369 (5)	0·3060 (5)	1·0031 (3)	0·050 (3)
N(4)	1·0149 (4)	0·2905 (4)	1·0931 (3)	0·050 (2)
C(5)	0·9085 (5)	0·3390 (5)	1·1106 (3)	0·054 (3)
C(6)	0·7571 (5)	0·2792 (5)	1·0279 (3)	0·051 (3)
C(11)	0·7149 (5)	0·3503 (4)	0·8740 (4)	0·047 (2)
O(11)	0·7646 (4)	0·3865 (3)	0·8123 (3)	0·062 (2)
C(12)	0·5755 (5)	0·3637 (4)	0·8784 (3)	0·044 (2)
C(13)	0·5576 (6)	0·4728 (4)	0·8631 (3)	0·046 (2)
C(14)	0·4219 (6)	0·4795 (5)	0·8556 (3)	0·048 (3)
O(14)	0·3915 (4)	0·5822 (3)	0·8419 (2)	0·062 (2)
C(15)	0·3027 (6)	0·3791 (5)	0·8585 (3)	0·047 (3)
O(15)	0·1662 (4)	0·3861 (3)	0·8469 (2)	0·059 (2)
C(16)	0·3223 (6)	0·2716 (5)	0·8748 (3)	0·048 (3)
O(16)	0·1997 (4)	0·1768 (3)	0·8779 (2)	0·057 (2)
C(17)	0·4586 (6)	0·2629 (4)	0·8849 (3)	0·048 (3)
C(18)	0·5086 (7)	0·6862 (5)	0·8354 (5)	0·090 (4)
C(19)	0·0791 (6)	0·3754 (5)	0·7497 (4)	0·070 (3)
C(20)	0·2258 (6)	0·0751 (5)	0·9138 (4)	0·064 (3)
C(21)	0·8284 (6)	0·1069 (4)	0·8926 (3)	0·056 (3)
O(22)	0·7132 (4)	0·0622 (3)	0·7973 (2)	0·062 (2)
C(23)	0·5683 (7)	0·0071 (5)	0·7894 (4)	0·062 (3)
O(23)	0·5296 (4)	−0·0085 (3)	0·8567 (3)	0·074 (2)
C(24)	0·4625 (7)	−0·0325 (6)	0·6850 (4)	0·080 (4)
C(25)	0·3052 (8)	−0·1021 (10)	0·6788 (6)	0·169 (6)
C(26)	0·4751 (12)	0·0849 (8)	0·6499 (6)	0·176 (7)
C(27)	0·5098 (9)	−0·1119 (7)	0·6257 (5)	0·125 (5)
C(41)	1·0863 (6)	0·2313 (5)	1·1499 (4)	0·050 (2)
O(41)	1·1426 (4)	0·1671 (3)	1·1182 (3)	0·064 (2)
C(42)	1·1032 (5)	0·2516 (4)	1·2534 (3)	0·050 (2)
C(43)	1·0889 (5)	0·1498 (5)	1·2952 (3)	0·057 (3)
C(44)	1·1167 (6)	0·1682 (5)	1·3917 (4)	0·066 (3)
O(44)	1·1051 (5)	0·0762 (4)	1·4411 (3)	0·096 (2)
C(45)	1·1629 (6)	0·2864 (5)	1·4482 (4)	0·071 (3)
O(45)	1·1885 (6)	0·3020 (4)	1·5446 (3)	0·102 (3)
C(46)	1·1791 (6)	0·3863 (5)	1·4050 (4)	0·071 (2)
O(46)	1·2276 (5)	0·4994 (4)	1·4658 (3)	0·111 (3)
C(47)	1·1475 (5)	0·3686 (5)	1·3077 (3)	0·060 (2)
C(48)	1·0454 (8)	−0·0479 (5)	1·3850 (4)	0·099 (4)
C(49)	1·3402 (9)	0·3424 (8)	1·6031 (5)	0·146 (6)
C(50)*	1·2479 (15)	0·5991 (11)	1·4311 (9)	0·142 (4)
C(50′)*	1·1007 (24)	0·5386 (20)	1·4910 (16)	0·142 (4)

* C(50) is disordered over two positions and is refined isotropically to take an occupancy of 63%. The congener is C(50′).

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, intramolecular bond angles, a full list of torsion angles and results of least-squares-planes calculations have been deposited with the British Library Document Supply Centre as Supplementary Publication No. 53724 (21 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

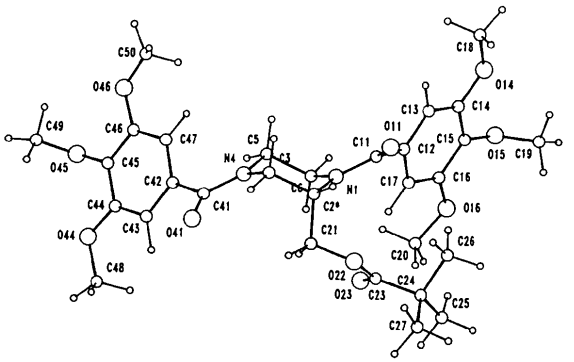

Fig. 1. A perspective drawing of the molecular structure with the atomic numbering scheme. The chair conformation of the piperazine ring is clearly indicated.

Table 2. *Intramolecular distances* (Å), *selected torsion angles* (°), *possible intermolecular hydrogen bonds and other contacts shorter than* 3·5 Å; *e.s.d.'s are given in parentheses*

N(1)—C(2)	1·459 (8)	C(21)—O(22)	1·450 (5)
N(1)—C(6)	1·476 (7)	O(22)—C(23)	1·347 (8)
N(1)—C(11)	1·366 (7)	C(23)—O(23)	1·202 (9)
C(2)—C(3)	1·526 (6)	C(23)—C(24)	1·522 (8)
C(2)—C(21)	1·518 (7)	C(24)—C(25)	1·489 (11)
C(3)—N(4)	1·456 (7)	C(24)—C(26)	1·514 (12)
N(4)—C(5)	1·461 (8)	C(24)—C(27)	1·517 (13)
N(4)—C(41)	1·359 (8)	C(41)—O(41)	1·233 (8)
C(5)—C(6)	1·523 (6)	C(41)—C(42)	1·498 (7)
C(11)—O(11)	1·229 (7)	C(42)—C(43)	1·398 (8)
C(11)—C(12)	1·498 (9)	C(42)—C(47)	1·376 (7)
C(12)—C(13)	1·396 (8)	C(43)—C(44)	1·369 (8)
C(12)—C(17)	1·396 (7)	C(44)—O(44)	1·373 (8)
C(13)—C(14)	1·379 (9)	C(44)—C(45)	1·396 (8)
C(14)—O(14)	1·373 (8)	O(44)—C(48)	1·430 (7)
C(14)—C(15)	1·386 (7)	C(45)—O(45)	1·372 (7)
O(14)—C(18)	1·419 (7)	C(45)—C(46)	1·390 (9)
C(15)—O(15)	1·376 (8)	O(45)—C(49)	1·400 (9)
C(15)—C(16)	1·388 (9)	C(46)—O(46)	1·372 (7)
O(15)—C(19)	1·427 (6)	C(46)—C(47)	1·376 (8)
C(16)—O(16)	1·372 (6)	O(46)—C(50)	1·314 (14)
C(16)—C(17)	1·387 (9)	O(46)—C(50′)	1·640 (30)
O(16)—C(20)	1·442 (8)		

N(1)—C(2)—C(3)—N(4)	50·8 (7)	C(3)—N(4)—C(41)—C(42)	160·5 (5)
C(2)—C(3)—N(4)—C(5)	−55·8 (7)	N(4)—C(41)—C(42)—C(43)	142·4 (6)
C(3)—N(4)—C(5)—C(6)	56·3 (7)	C(11)—N(1)—C(2)—C(21)	−113·2 (6)
N(4)—C(5)—C(6)—N(1)	−52·1 (7)	N(1)—C(2)—C(21)—O(22)	71·4 (6)
C(5)—C(6)—N(1)—C(2)	51·9 (7)	C(2)—C(21)—O(22)—C(23)	−106·9 (6)
C(6)—N(1)—C(2)—C(3)	−50·8 (7)	C(21)—O(22)—C(23)—C(24)	179·2 (6)
C(2)—N(1)—C(11)—O(11)	−11·4 (9)	O(22)—C(23)—C(24)—C(25)	175·3 (7)
C(2)—N(1)—C(11)—C(12)	164·4 (6)	O(22)—C(23)—C(24)—C(26)	−65·6 (8)
N(1)—C(11)—C(12)—C(13)	143·9 (6)	O(22)—C(23)—C(24)—C(27)	53·4 (8)
C(3)—N(4)—C(41)—O(41)	−16·0 (10)		

D—H*···*A*	H···*A*	*D*···*A*	*D*—H···*A*	Symmetry†
C(2)—H(2)···O(15)	2·531 (7)	3·279 (7)	125·6 (5)	$x+1, y, z$
C(3)—H(3*B*)···O(16)	2·463 (7)	3·411 (8)	145·8 (5)	$x+1, y, z$
C(6)—H(6*A*)···O(14)	2·475 (7)	3·409 (8)	144·1 (5)	$1-x, 1-y, 2-z$
C(3)···O(15)		3·099 (7)		$x+1, y, z$
C(18)···O(41)		3·166 (8)		$2-x, 1-y, 2-z$
C(21)···O(41)		3·444 (8)		$2-x, -y, 2-z$

*H atom in calculated position, 1·08 Å from the parent atom.
†The symmetry translation code refers to the second non-H atom.

C—N—C angles are 116·0 (5) [113·6 (5)°]. The mean values within the piperazine ring are: C—N = 1·468 [1·458] Å and C—C = 1·524 Å. Further, the N atoms which are located on each side of the central piperazine carbon plane, C(2)C(3)C(5)C(6), deviate from the plane by 0·56 (1) and [0·61 (1)] Å, respectively.

The conformation of the side chain is of interest when discussing the receptor stereospecificity. The *tert*-butylcarboxymethyl side chain is almost perpendicularly attached to the C(2) atom of the piperazine nucleus as described by the torsion angles C(11)—N(1)—C(2)—C(21) and N(1)—C(2)—C(21)—O(22), −113·2 (6) and 71·4 (6)°, respectively. The remaining main torsion angles of the side chain C(2)—C(21)—O(22)—C(23) and C(21)—O(22)—C(23)—C(24) are −106·9 (6) and 179·2 (6)°, directing the tail away from the piperazine ring.

The weighted least-squares planes through the six-membered rings of the piperazine and the two trimethoxyphenyl moieties are oriented almost perpendicular to each other. The dihedral angle between the piperazine and benzene planes is 80·2 (2) [80·1 (2)]° and the angle between the two benzene planes is 84·5 (2)°. The methoxy O atoms show small deviations from the plane of the benzene rings and have mean deviation values ±0·034 [±0·031] Å. Two of the methoxy C atoms are also located essentially within each benzene plane, deviating less than ±0·274 [±0·141] Å. Only the displacement of the central methoxy C atom is more pronounced, being 1·393 (6) [1·214 (11)] Å.

The amide moieties are essentially planar. The displacements of the atoms from the planes defined by C(6)N(1)C(2)C(11)O(11)C(12) and C(3)N(4)C(5)C(41)O(41)C(42) are of the same order and in each case less than 0·22 Å. These facts speak in favor of a limited flexibility of the amide groups. The angle between the planes is 19·9 (2)°. The observed amide distances are N—C(carbonyl) = 1·366 (7) [1·359 (8)]; C=O = 1·229 (7) [1·233 (8)] and C(carbonyl)—C(phenyl) = 1·498 (9) [1·498 (7)] Å.

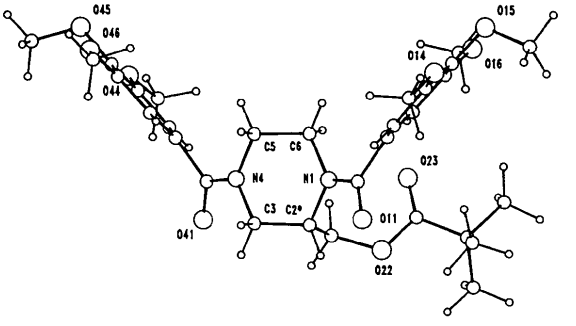

Fig. 2. Molecular view of the *S* conformer, viewed perpendicular to the piperazine plane. The distance O15–O45 = 12·75 Å and O11–O41 = 6·44 Å. The pseudo-twofold axis runs through the midpoint of the piperazine ring and is oriented parallel to the vertical axis of the paper.

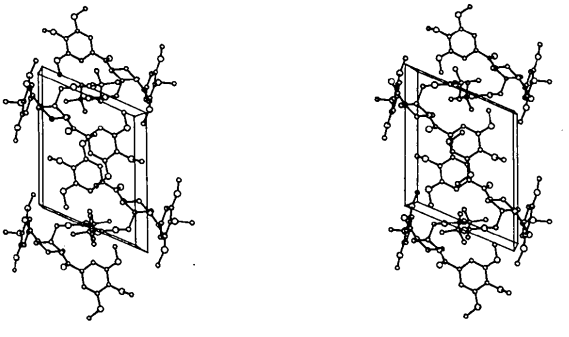

Fig. 3. Stereoscopic view, illustrating the crystal packing viewed down the *c* axis. The piperazine and two trimethoxyphenyl rings are oriented almost parallel to the coordinate planes of the unit cell. The molecules are mainly held together by van der Waals forces. Large open circles represent the O atoms. The H atoms are omitted for clarity. The view has the origin at the lower left corner, the *a* axis nearly horizontal and the *b* axis vertical to the plane of the paper.

The mean distances within the trimethoxyphenyl moieties are C—C = 1·389 [1·384] Å and the average values within the three methoxy groups are C—O = 1·374 [1·372] Å and O—CH_3 = 1·429 [1·446] Å, respectively.

Crystal packing. The packing scheme of the crystal structure is shown in Fig. 3, viewed along the crystallographic *c* axis. The piperazine and trimethoxyphenyl rings are mainly oriented parallel to the coordinate planes of the unit cell. The predominant stabilizing forces between adjacent molecules are likely to be of van der Waals character, but from the molecular packing a conceivable weak π-electron overlap between adjacent trimethoxyphenyl moieties is also expected. A detailed scheme involving distances less than 3·5 Å is found in Table 2. Only a few possible weak hydrogen bonds are found, involving three C atoms of the piperazine ring loosely bonded to three O atoms of a neighbouring trimethoxyphenyl moiety attached to N(1). No hydrogen bonding or short interaction is found which includes the O atoms of the other pseudo-related trimethoxyphenyl moiety. The side chain is stabilized by a short interaction between C(21) and the carbonyl O(41) in an adjacent molecule.

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Structure of Methyl 1,3-Dihydro-4-methyl-3-oxofuro[3,4-*b*]pyridin-1-ylacetate

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(*Received* 10 *September* 1990; *accepted* 2 *November* 1990)

Abstract. $C_{11}H_{11}NO_4$, M_r = 221, monoclinic, $P2_1/c$, a = 10·28 (1), b = 15·45 (3), c = 6·752 (2) Å, β = 95·88 (6)°, V = 1066 (4) Å^3, Z = 4, D_x = 1·378 g cm^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, μ = 8·52 cm^{-1}, $F(000)$ = 464, T = 298 K, R = 0·056 for 1008 observed reflexions. The bicyclic ring system of the title lactone (2) is essentially flat, the nine atoms of the ring system, together with substituent methyl C and carbonyl O atoms, lying within 0·047 Å of their least-squares best plane. The C and O atoms of

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0108-2701/91/071457-04$03.00