

corrélations  $r$  suivantes:  $r(\alpha, d_6) = 0,93$  et  $r(\alpha, d'_6) = -0,70$ . En d'autres termes, plus le système tricyclique se plie, plus la distance entre les substituants en *cis-exo* se rapprochent et ceux en *cis-endo* s'éloignent (cas du *cis-DA* et du fluotrène).

— Contraintes des substituants avec les *péri*-atomes d'hydrogène [H(1), H(4), H(6), H(9)]. Un calcul des distances  $d_2, d'_2, d_3, d'_3, d_4, d'_4, d_5, d'_5$  (Fig. 1) montre qu'elles sont du même ordre que celles de van der Waals. La présence d'un centre de symétrie cristallin pour l'ensemble de ces composés rend compte de l'équivalence des atomes en position H1, H4, H6 et H9. Afin d'établir des corrélations il semble préférable d'effectuer une moyenne entre les distances équivalentes ( $d_2, d'_2, d_4, d'_4$  notée  $d_{m1}$ ) et ( $d_3, d'_3, d_5, d'_5$  notée  $d_{m2}$ ). Il apparaît comme attendu les corrélations suivantes:  $r(\alpha, d_{m1}) = -0,83$  et  $r(\alpha, d_{m2}) = -0,92$ . En d'autres termes un pliage du système tricyclique accroît les distances  $d_m$  et place donc les substituants en position *exo* du système tricyclique.

Ce type de contrainte a pour effet de placer le ou les substituants dans une position de fuite (équatoriale) et ainsi de fermer le tricycle (cas du *trans-DA*).

Dans le cas de la tacitine et de son dérivé *N*-méthylé, le pontage éthane du cycle central a pour effet de renforcer le contact du type  $d_6$  et par conséquent de plier davantage le système tricyclique ( $\alpha = 118^\circ$ ).

Pendant que cet article était soumis à *Acta Crystallographica*, la structure de ce composé est parue dans ce même journal (Herbstein, Kapon & Reisner, 1986).

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## Stereoelectronic Effects in Oxidative Transformations of Purines. I. Structure of 4,5-Dihydro-4,5-dimethoxy-1-methyluric Acid\*

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**Abstract.**  $C_8H_{12}N_4O_5$ ,  $M_r = 244.21$ , monoclinic,  $P2_1/c$ ,  $a = 12.259$  (8),  $b = 7.021$  (5),  $c = 12.074$  (5) Å,  $\beta = 97.62$  (4)°,  $V = 1030$  (1) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.575$  g cm<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.7107$  Å,  $\mu = 1.42$  cm<sup>-1</sup>,  $F(000) = 512$ , room temperature,  $R = 0.060$  for 1593

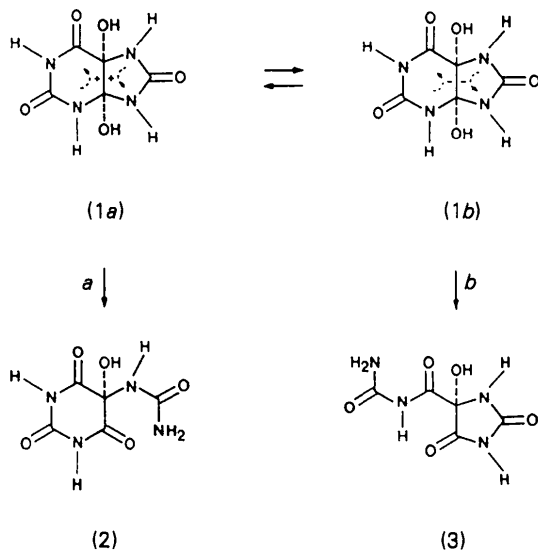
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observed reflections. The *cis*-fused bicyclic system has a distinct ring-twisted conformation defined by the bridgehead torsion angle C(6)–C(5)–C(4)–N(9) of  $-91.8$  (4)°. The orthogonal C(2)–N(3)–C(4)–N(9) array [89.0 (5)°] with N(3) antiperiplanar to the 4-methoxy group allows the cleavage of the C(4)–N(9) bond to take place with stereoelectronic control.

\* Uric acid is 7,9-dihydro-1*H*-purine-2,6,8(3*H*)-trione.

**Introduction.** The application of the stereoelectronic theory (Deslongchamps, 1984) to the cleavage of tetrahedral intermediates in uricolytic processes may explain some long-standing anomalies in chemical and enzymic reactions. The ring fission of the tetrahedral intermediate (1) at the 3,4-bond (path *b*) constitutes the key step of the caffolide pathway, which is, besides the allantoin pathway, the main route for biological degradation of purines (Poje, Paulus & Ročić, 1980; Poje, Palković, Perina, Vicković & Bruvo, 1985). However, alloxan-like products (2) formed by an alternative ring fission at the 4,9-bond (path *a*) exerted strong cytotoxic effects upon  $\beta$  cells of rat pancreatic islets of Langerhans, which led to a plausible hypothesis that aberrations in purine metabolism could have relevance to the aetiology of diabetes mellitus (Poje & Ročić, 1979, 1980; Poje, Ročić, Sikirica, Vicković & Bruvo, 1983).



On the basis of the stereoelectronic principle, the orientation in space of the non-bonded electron pairs in tetrahedral intermediate (1) is crucial to an understanding of the regioselective cleavage at C(4). In flexible *cis*-fusion, the signs of the torsion angles of the junction can be simultaneously inverted, giving two conformational isomers (1*a*) and (1*b*). This implies that a conformational change (1*a*) $\rightleftharpoons$ (1*b*) acts as a switch controlling the mode of cleavage. In order to confirm and to obtain a more detailed knowledge of such a mechanism, precise information is required on the structure and stereochemistry of intermediate (1). Normally, this information can be obtained only indirectly because this intermediate is a transient species. Using this approach we have examined a model of (1*a*), 4,5-dihydro-4,5-dimethoxy-1-methyluric acid, which undergoes a regiospecific ring opening at the 4,9-bond (path *a*).

**Experimental.** The title compound was prepared by chlorination of 1-methyluric acid in cold anhydrous methanol. Recrystallization from water gave colourless plates. Crystal dimensions 0.23  $\times$  0.23  $\times$  0.50 mm, automated four-circle Philips PW 1100 diffractometer, graphite-monochromatized Mo  $K\alpha$  radiation, cell parameters from 14 reflections ( $7 \leq \theta \leq 10^\circ$ ). Intensity data were collected in the usual  $\theta$ - $2\theta$  scan mode, scan width  $1.8^\circ$ , scan speed  $0.06^\circ \text{ s}^{-1}$ . From 2229 independent reflections ( $-17 \leq h \leq 17$ ,  $0 \leq k \leq 9$ ,  $0 \leq l \leq 16$ ,  $6.7 \leq 2\theta \leq 60.0^\circ$ ), 277 reflections with  $I \leq 3\sigma(I)$ , 354 with poor  $F_o/F_c$  agreement having  $F_o \leq 0.031(F_o)_{\text{max}}$ , and five reflections (110, 002, 202, 212,  $\bar{1}12$ ) due to the secondary extinction were ignored. Three standard reflections showed no significant variation in intensity. Lorentz-polarization (locally written program) and absorption correction (Harkema, 1978) with transmission factor 0.960–0.973 were applied. Direct methods (MULTAN80, Main *et al.*, 1980) gave all C, N, O atomic positions, ten H atoms located from  $\Delta F$  map determined the best positions of all H atoms (Vicković, 1985). At the end of non-H refinement, ureide H atoms were relocated by a  $\Delta F$  synthesis in order to confirm their specific geometry. Final refinement included the coordinates of all atoms, except H atoms of the C(11) atom, anisotropic thermal parameters of non-H atoms and isotropic thermal parameters of H atoms; 1593 observed intensity data and 193 parameters in full-matrix least-squares procedure (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976),  $\sum w(|F_o| - |F_c|)^2$  minimized,  $w = \sigma^{-2}(F_o)$ ,  $(\sin \theta / \lambda)_{\text{max}} = 0.56 \text{ \AA}^{-1}$ ; scattering factors for C, N, O (Cromer & Mann, 1968) and for H (Stewart, Davidson & Simpson, 1965), and corrections for anomalous-dispersion effects for non-H atoms (Cromer & Liberman, 1970) led to a final  $R = 0.060$ ,  $wR = 0.077$ ,  $S = 2.95$ ,  $(\Delta/\sigma)_{\text{max}} = 1.05$ ,  $(\Delta/\sigma)_{\text{av}} = 0.07$  for all refined parameters. Highest peak in final  $\Delta F$  map  $\Delta\rho_{\text{max}} = 0.49 \text{ e \AA}^{-3}$ . All calculations were carried out using a Univac 1110/42 computer.

**Discussion.** Final atomic coordinates and equivalent isotropic thermal parameters are given in Table 1,\* main bond lengths and angles and hydrogen-bond geometry in Table 2. An ORTEP drawing (Johnson, 1971) of the molecule is shown in Fig. 1 with the numbering scheme and the hydrogen-bonding pattern.

The molecular structure shows a ring-twisted conformation of the *cis*-fused bicyclic system defined by the bridgehead torsion angle C(6)–C(5)–C(4)–N(9) of  $-91.8(4)^\circ$ , which corresponds to the conformer (1*a*).

\* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond distances and angles involving H atoms and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43418 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The most important conformational feature is the virtually orthogonal C(2)—N(3)—C(4)—N(9) array [89.0 (5)°]; a similar situation holds for the H(3)—N(3)—C(4)—N(9) torsion angle of -89 (3)°. The glycol ether grouping [O(4)—C(4)—C(5)—O(5) 25.3 (4)°] has a *gauche* conformation for methyl C(10) and an *anti* conformation for C(11) with respect to the

C(4)—C(5) bond. Significantly, the 4-methoxy substituent is oriented antiperiplanar to the N(3)—C(4) bond; the arrangement of the 4-methoxy group with respect to the bicyclic system is such that there is a shorter N(9)⋯C(10) contact of 2.830 (7) Å (the sum of van der Waals radii being 3.35 Å). The N atoms of the five-membered ring show considerable deviations from planarity; the distances of N(7) and N(9) from the planes through their adjacent atoms are 0.263 (3) and -0.191 (3) Å, respectively.

Table 1. Fractional atomic coordinates ( $\times 10^4$ ) and  $U_{eq}$  ( $\text{Å}^2 \times 10^3$ ) values

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{eq}^\dagger$
N(1)	3788 (3)	5873 (5)	10653 (3)	37 (1)
C(1)	4419 (5)	4768 (10)	11563 (5)	56 (1)
C(2)	4158 (3)	7726 (6)	10462 (3)	37 (1)
O(2)	5049 (3)	8240 (5)	10920 (3)	54 (1)
N(3)	3492 (3)	8836 (6)	9763 (3)	42 (1)
C(4)	2412 (3)	8384 (6)	9219 (3)	31 (1)
O(4)	2357 (2)	9369 (4)	8207 (2)	39 (1)
C(5)	2255 (3)	6202 (6)	9099 (3)	32 (1)
O(5)	2573 (3)	5719 (5)	8064 (3)	48 (1)
C(6)	2922 (3)	5025 (6)	10025 (3)	32 (1)
O(6)	2658 (2)	3379 (5)	10176 (3)	45 (1)
N(7)	1099 (3)	5957 (5)	9220 (3)	35 (1)
C(8)	743 (3)	7497 (6)	9761 (3)	33 (1)
O(8)	-156 (2)	7603 (4)	10116 (3)	49 (1)
N(9)	1530 (3)	8869 (5)	9849 (3)	33 (1)
C(10)	1326 (4)	9372 (9)	7505 (5)	52 (1)
C(11)	2313 (6)	3876 (8)	7656 (5)	70 (2)

$$\dagger U_{eq} = \frac{1}{3} \{ U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aba^*b^*c\cos\gamma + 2U_{13}aca^*c^*\cos\beta + 2U_{23}bcb^*c^*\cos\alpha \}$$

Table 2. Bond lengths (Å) and angles (°) and geometry of the hydrogen bonds (*e.s.d.*'s in parentheses)

N(1)—C(1)	1.477 (7)	O(4)—C(10)	1.425 (5)	
N(1)—C(2)	1.407 (6)	C(5)—O(5)	1.399 (5)	
N(1)—C(6)	1.358 (5)	C(5)—C(6)	1.536 (5)	
C(2)—O(2)	1.212 (5)	C(5)—N(7)	1.454 (5)	
C(2)—N(3)	1.343 (5)	O(5)—C(11)	1.406 (7)	
N(3)—C(4)	1.433 (5)	C(6)—O(6)	1.220 (5)	
C(4)—O(4)	1.398 (5)	N(7)—C(8)	1.364 (6)	
C(4)—C(5)	1.548 (6)	C(8)—O(8)	1.237 (5)	
C(4)—N(9)	1.443 (6)	C(8)—N(9)	1.358 (5)	
C(1)—N(1)—C(2)	117.3 (4)	C(4)—C(5)—C(6)	114.6 (3)	
C(1)—N(1)—C(6)	118.6 (4)	C(4)—C(5)—N(7)	102.6 (3)	
C(2)—N(1)—C(6)	124.0 (3)	O(5)—C(5)—C(6)	109.6 (3)	
N(1)—C(2)—O(2)	119.4 (4)	O(5)—C(5)—N(7)	116.9 (3)	
N(1)—C(2)—N(3)	117.2 (4)	C(6)—C(5)—N(7)	107.2 (3)	
O(2)—C(2)—N(3)	123.4 (4)	C(5)—O(5)—C(11)	117.3 (4)	
C(2)—N(3)—C(4)	127.4 (4)	N(1)—C(6)—C(5)	118.2 (3)	
N(3)—C(4)—O(4)	103.0 (3)	N(1)—C(6)—O(6)	122.4 (4)	
N(3)—C(4)—C(5)	111.0 (3)	C(5)—C(6)—O(6)	119.5 (3)	
N(3)—C(4)—N(9)	114.7 (3)	C(5)—N(7)—C(8)	109.4 (3)	
O(4)—C(4)—C(5)	114.6 (3)	N(7)—C(8)—O(8)	124.7 (4)	
O(4)—C(4)—N(9)	113.0 (3)	N(7)—C(8)—N(9)	109.3 (3)	
C(5)—C(4)—N(9)	101.0 (3)	O(8)—C(8)—N(9)	125.9 (4)	
C(4)—O(4)—C(10)	117.2 (3)	C(4)—N(9)—C(8)	111.5 (3)	
C(4)—C(5)—O(5)	106.1 (3)			
N—H⋯O	N—H	H⋯O	N⋯O	N—H⋯O
N(3)—H(3)⋯O(2 <sup>i</sup> )	0.89 (5) Å	2.10 (4) Å	2.913 (6) Å	151 (4)°
N(7)—H(7)⋯O(8 <sup>ii</sup> )	0.89 (4)	2.04 (4)	2.911 (5)	165 (3)
N(9)—H(9)⋯O(8 <sup>iii</sup> )	0.86 (4)	2.23 (4)	2.999 (5)	150 (3)

Symmetry codes: (i) 1-x, 2-y, 2-z; (ii) -x, 1-y, 2-z; (iii) x, 1/2-y, -1/2+z.

The compound is hydrolyzed spontaneously and the crystal structure shows that differences in bond lengths and angles are already present in the ground state. A comparison of C—N bonds in the ester aminal function shows no significant difference in bond length between the cleaving C(4)—N(9) bond and the N(3)—C(4) bond, the latter being somewhat shortened in comparison with that in the related 4,5-dihydro-4,5-dimethoxy-3,7-dimethyluric acid (Poje & Vicković, 1987). However, the O atom with an electron pair antiperiplanar to the C(4)—N(9) bond definitely has a larger O(4)—C(4)—N(9) angle than the N(3)—C(4)—O(4) angle of the ester aminal function. These differences in bond lengths and angles suggest a description in which the non-bonding electrons are delocalized by mixing with the suitably oriented antibonding  $\sigma$  orbital of the C(4)—N(9) bond; the developing *p* orbitals on N and O must be parallel in the transition state, and this means that the lone-pair orbitals on N and O, and the C—N bond must all lie parallel (Fig. 2). This type of delocalization will strengthen the N(3)—C(4) bond and will weaken the C(4)—N(9) bond.

By assuming that conformational properties are retained in solution, and that rapid expulsion of any substituent from the ester aminal function requires the proper electron-pair orientation, we nicely account for the cleavage at the C(4)—N(9) bond (path *a*) and the absence of concurrent N(3)—C(4) bond cleavage (path *b*) in acidic hydrolysis of 4,5-dihydro-4,5-dimethoxy-1-methyluric acid.

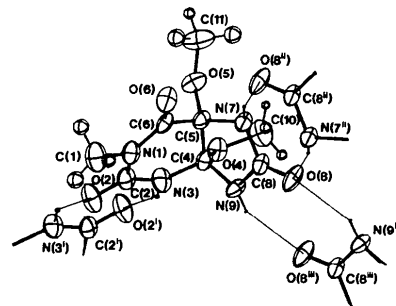


Fig. 1. Molecular conformation of the title compound (*R,R*-configuration) showing 50% probability thermal ellipsoids.

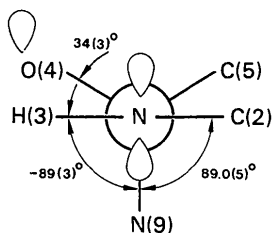


Fig. 2. The Newman projection along the N(3)–C(4) axis showing the alignment of non-bonded electron pairs and the cleaving C(4)–N(9) bond in the ester aminal function; N and O electron escorts are pictured as  $sp^2$ - and  $sp^3$ -hybridized, respectively.

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## Stereoelectronic Effects in Oxidative Transformations of Purines. II. Structure of 4,5-Dihydro-4,5-dimethoxy-3,7-dimethyluric Acid\*

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(Received 7 February 1986; accepted 17 September 1986)

**Abstract.**  $C_9H_{14}N_4O_5$ ,  $M_r = 258.24$ , triclinic,  $P\bar{1}$ ,  $a = 12.443(6)$ ,  $b = 7.508(4)$ ,  $c = 6.883(4)$  Å,  $\alpha = 107.60(4)$ ,  $\beta = 91.56(5)$ ,  $\gamma = 100.05(3)^\circ$ ,  $V = 601.3(5)$  Å<sup>3</sup>,  $Z = 2$ ,  $D_x = 1.426$  g cm<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.7107$  Å,  $\mu = 1.26$  cm<sup>-1</sup>,  $F(000) = 272$ , room temperature,  $R = 0.038$  for 2478 observed reflections. Substitution at N(7) causes steric overcrowding which favours the ring-twisted conformation of the *cis*-fused bicyclic system defined by the bridgehead torsion angle N(3)–C(4)–C(5)–N(7) of  $92.0(1)^\circ$ . The nearly orthogonal N(3)–C(4)–N(9)–C(8) array [ $-95.3(1)^\circ$ ]

with N(9) antiperiplanar to the 4-methoxy group allows the cleavage of the N(3)–C(4) bond to take place with stereoelectronic control.

**Introduction.** The crystal-structure determination of the title compound was undertaken in continuation of our studies of conformational properties of tetrahedral intermediates in oxidative transformations of purines. We felt that the knowledge of bond-breaking processes and the required conformational changes of specific enzyme transformations could be gained through the application of stereoelectronic principles (Deslongchamps, 1984).

\* Uric acid is 7,9-dihydro-1*H*-purine-2,6,8(3*H*)-trione.