

Discussion. A view of the molecule showing its conformation and the numbering system is presented in Fig. 1; Fig. 2 is a stereoscopic view [figures drawn using *ORTEP* (Johnson, 1965)]. All intermolecular distances and angles were computed and evidence was found for hydrogen bonding. Crystalline cohesion seems to be due to hydrogen bonds as for MGBG, where parallel planar molecules are tied together by hydrogen bonds through water and Cl⁻ ions (Hamilton & La Placa, 1968). Atomic positional parameters are reported in Table 1. The intramolecular bond distances and angles are reported in Table 2.

Our study shows that in (5) and (6) the amidinohydrazone groups both have a *trans* conformation (*E*); however, these groups differ notably in their relative position on the pyrazole ring. The visualization of this difference offers a definite proof of the respective structures of these isomers and sustains the value of the chemical and NMR data hitherto put forward to characterize them.

The comparison of the three-dimensional structures of (5), (6) (Cousson, Robert & Hubert-Habart, 1990) and MGBG (Hamilton & La Placa, 1968) shows that pyrazole (6) is more closely related to MGBG than pyrazole (5). This could help to interpret the fact that the first two are good inhibitors of the enzyme *S*-adenosylmethioninedecarboxylase (SAMDC, 4.1.1. 50; *Enzyme Nomenclature*, 1978; Porter, Dave & Mihich, 1981), while the last one is

much less so (Mamont, 1989). Extension of such a type of observation should help in designing analogues of MGBG with more satisfactory anti-cancer activity.

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Camphoric Acid and Ammonium Hydrogen Camphorate Monohydrate

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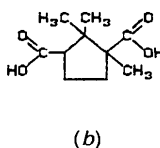
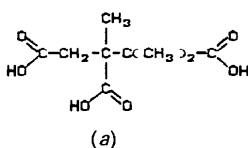
Abstract. (I) C₁₀H₁₆O₄, *M_r* = 200.23, monoclinic, *P*2₁, *a* = 13.107 (12), *b* = 11.828 (8), *c* = 7.740 (6) Å, β = 109.93 (6)°, *V* = 1128.06 Å³, *Z* = 4, *D_x* = 1.18 g cm⁻³, λ(Mo *K*α) = 0.71069 Å, μ = 0.28 cm⁻¹, *F*(000) = 432, *T* = 293 K, *R* = 0.069 for 1283 reflexions. (II) C₁₀H₁₆O₄, *M_r* = 200.23, orthorhombic, *P*2₁2₁2₁, *a* = 16.31 (3), *b* = 13.372 (4), *c* =

11.486 (2) Å, *V* = 2505.06 Å³, *Z* = 8, *D_x* = 1.06 g cm⁻³, λ(Mo *K*α) = 0.71069 Å, μ = 0.59 cm⁻¹, *F*(000) = 864, *T* = 293 K, 665 reflexions, disordered structure, refinement unsatisfactory. (III) NH₄⁺ · C₁₀H₁₅O₄⁻ · H₂O, *M_r* = 235.28, trigonal, *P*3₂, *a* = 13.013 (5), *c* = 6.326 (7) Å, *V* = 927.71 Å³, *Z* = 3, *D_x* = 1.26 g cm⁻³, λ(Mo *K*α) = 0.71069 Å, μ = 0.94 cm⁻¹, *F*(000) = 384, *T* = 293 K, *R* = 0.080 for 960 reflexions. Several crystalline forms of camphoric

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acid have been prepared. Both (I) and (II) contain hydrogen-bonded chains [O...O 2.640 (6) Å], ordered in (I) but disordered in (II). In (III) the carboxylate groups, ammonium ions and water molecules form a helical hydrogen-bonding system about a threefold axis.

Introduction. The structure of tricarballic acid was reported recently (Barnes & Paton, 1988) as one of a series of studies of polycarboxylate ligands and their complexes (Barnes & Paton, 1982, 1984). An attempt to prepare camphoric acid (2,3-dimethyl-1,2,3-tricarboxylic acid) (*a*), a trimethyl analogue of tricarballic acid, by a traditional destructive oxidation of camphor yielded the intermediate stage, camphoric acid (1,2,2-trimethyl-1,3-cyclopentanedicarboxylic acid) (*b*). Camphoric acid has several forms, one is reported in detail and a second in outline along with the structure of an ammonium salt.



Experimental. Following Goebel & Noyes (1923), camphor was oxidized with boiling concentrated nitric acid for four weeks. The major product was camphoric acid. Several different crystal forms were obtained from different solvents. Of these (I), obtained from water and from ethanol, gave the best diffraction pattern and was selected for study. A brief account of the extensively disordered (II), from acetone, is given below. Partial neutralization of (I) with aqueous ammonia gave (III), which proved to be ammonium hydrogen camphorate monohydrate.

After preliminary photographs, data for all three compounds were collected on a Stoe STADI II diffractometer using crystals mounted in Lindemann-glass capillaries. The crystals of (I) were obtained from aqueous solution. Crystals showed no significant change in the intensities of standard reflections during data collection. Unit-cell dimensions were refined from 15–20 accurately centred reflections with $\theta \approx 12^\circ$. Data were also collected for a crystal of (I) (from ethanol) on a Nicolet P3 diffractometer. The coordinates *etc.* reported for (I) are derived from this data set unless specifically mentioned. In this case the cell was refined using the angles of 20 accurately centred reflections in the range $15 \leq 2\theta \leq 18^\circ$. Data were corrected for the Lorentz and polarization terms but not for absorption. The structures were solved by direct methods and refined by routine least-squares procedures and difference syntheses. Programs used included *SHELXS* (Sheldrick, 1986),

SHELX76 (Sheldrick, 1976), *XANADU* (Roberts & Sheldrick, 1975) and *PLUTO* (Motherwell & Clegg, 1978). Atomic scattering factors from *SHELX76*.

(I) A crystal $0.30 \times 0.65 \times 0.50$ mm was mounted near the *ac* diagonal. ω - θ scan. Data were collected for a quadrant of reciprocal space for $1 \leq \theta \leq 25^\circ$. 2243 measured reflexions gave 2085 unique data ($R_{\text{int}} = 0.037$) of which 1283 with $|F_o| \geq 4\sigma(F)$ were used in the final refinement. Ranges of indices $-15 \leq h \leq 15$, $0 \leq k \leq 14$, $0 \leq l \leq 9$.

Routine refinement led to convergence with anisotropic temperature parameters for all non-H atoms. All H atoms were placed on calculated positions with isotropic temperature parameters fixed at 0.15 \AA^2 except for the acid protons which were omitted. Final refinement (minimizing $\sum w|F_o - |F_c||^2$), 252 refined parameters, $R = 0.069$, $wR = 0.89$, $w = 1.5055/[\sigma(F)^2 + 0.001795F^2]$, mean shift/e.s.d. = 0.022 , max. shift/e.s.d. = 0.051 , max. difference peak = 0.238 e \AA^{-3} , max. negative peak = $-0.196 \text{ e \AA}^{-3}$.

The data set from the STADI II diffractometer refined to $R = 0.068$, $wR = 0.090$ for 1329 unique reflexions with $F \geq 3\sigma(F)$. The atomic coordinates were all within 2σ of those reported below; the temperature factors showed a very similar pattern but were consistently small by about 5%.

(II) Several crystals were examined from the limited supply which was available, all diffracted only weakly. A crystal $0.53 \times 0.38 \times 0.36$ mm was mounted on the *a* axis. ω scan. Data were collected for a hemisphere of reciprocal space for $1 \leq \theta \leq 25^\circ$. Significant counts were obtained for only 1202 of the 4607 reflexions measured, giving 668 unique data ($R_{\text{int}} = 0.045$). Ranges of indices $0 \leq h \leq 16$, $-11 \leq k \leq 11$, $-12 \leq l \leq 12$. Although a chemically reasonable, partially disordered, model was obtained from the limited data available, refinement was abandoned as unsatisfactory after extensive studies of site occupancies using rigid models for the molecule, based on (I), to simulate ill defined regions of the structure. The main features of the model are discussed below.

(III) A crystal $0.27 \times 0.38 \times 0.72$ mm was mounted on the *c* axis. Weissenberg photographs for layers *hk0* and *hk1* showed the relationships expected for a trigonal system (Buerger, 1942). The intensity pattern and systematic absences (*International Tables for X-ray Crystallography*, 1969, Vol. I) and the value $Z = 3$ predicted from the density were consistent with the chosen space group, which yielded a satisfactory model.

Data were collected for a hemisphere of reciprocal space for $1 \leq \theta \leq 25^\circ$. ω scan. 3616 measured reflexions gave 1178 unique data ($R_{\text{int}} = 0.040$) of which 960 with $|F_o| \geq 3\sigma(F)$ were used in the final refinement. Ranges of indices $-15 \leq h \leq 15$, $-15 \leq k \leq 15$, $0 \leq l \leq 6$.

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic thermal parameters ($\times 10^3$) for non-H atoms of (I)
$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	U_{eq} (\AA^2)
C1	5193 (5)	4591 (6)	-1338 (8)	68 (2)
C2	4855 (5)	5190 (7)	-3244 (8)	68 (2)
C3	3681 (5)	4710 (7)	-4125 (8)	78 (2)
C4	3210 (5)	4688 (8)	-2551 (8)	84 (2)
C5	4139 (5)	4543 (10)	-838 (9)	103 (3)
C6	5649 (7)	3405 (8)	-1356 (12)	116 (3)
C7	6068 (5)	5239 (7)	133 (8)	72 (2)
O8	7016 (4)	5267	-34 (6)	102 (2)
O9	5893 (4)	5733 (6)	1387 (6)	103 (2)
C10	4813 (7)	6501 (8)	-3029 (10)	106 (3)
C11	5581 (5)	4963 (9)	-4366 (9)	97 (3)
C12	2990 (6)	5360 (9)	-5818 (9)	91 (3)
O13	3234 (5)	5263 (7)	-7261 (6)	119 (2)
O14	2221 (5)	5923 (8)	-5806 (7)	151 (3)
C21	561 (5)	7684 (6)	-1768 (8)	64 (2)
C22	-533 (5)	7005 (6)	-2738 (7)	56 (2)
C23	-888 (5)	7545 (6)	-4665 (7)	64 (2)
C24	135 (6)	7787 (8)	-5076 (10)	89 (2)
C25	1071 (5)	7795 (8)	-3250 (8)	82 (2)
C26	300 (7)	8859 (8)	-1177 (11)	108 (3)
C27	1285 (5)	7039 (8)	-91 (8)	80 (2)
O28	1021 (5)	7130 (7)	1344 (7)	138 (3)
O29	2073 (4)	6509 (6)	-99 (6)	98 (2)
C30	-274 (6)	5751 (7)	-2914 (9)	92 (3)
C31	-1362 (5)	7103 (10)	-1784 (9)	103 (3)
C32	-1720 (5)	6866 (7)	-6096 (8)	66 (2)
O33	-2691 (4)	6842 (6)	-5953 (7)	101 (2)
O34	-1517 (4)	6351 (6)	-7309 (6)	101 (2)

Routine refinement led to convergence using anisotropic temperature parameters for all non-H atoms. H atoms were placed on calculated positions with refined isotropic temperature parameters except for two of the ammonium H atoms which were located on a difference map, the acid H atom on O8 and the water H atoms which were not included. The relatively high value of R (0.080) was probably due to poor peak quality, associated with the large crystal used to maximize intensity. Final refinement (minimizing $\sum w|F_o - |F_c||^2$), 148 refined parameters, $R = 0.080$, $wR = 0.082$, $w = 5.4402/[\sigma(F)^2 + 0.000360F^2]$, mean shift/e.s.d. = 0.002, max. shift/e.s.d. = 0.003, max. difference peak = 0.297 e \AA^{-3} , max. negative peak = -0.395 e \AA^{-3} .

Discussion. Final atomic coordinates for (I) and (III) are given in Tables 1 and 3 with bond lengths and angles in Tables 2 and 4,* respectively. The numbering scheme is shown in Fig. 1.

In (I) molecules are linked together by four hydrogen bonds [2.644 (6) \AA], to form infinite folded chains, Fig. 2. These chains are normal to the b axis

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53970 (19 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. Interatomic distances (\AA) and angles ($^\circ$) and hydrogen-bond lengths (\AA) for (I)

C2—C1	1.558 (9)	C5—C1	1.557 (10)
C6—C1	1.527 (12)	C7—C1	1.520 (9)
C3—C2	1.561 (9)	C10—C2	1.563 (12)
C11—C2	1.515 (11)	C4—C3	1.543 (10)
C12—C3	1.523 (10)	C5—C4	1.473 (8)
O8—C7	1.293 (9)	O9—C7	1.220 (9)
O13—C12	1.268 (10)	O14—C12	1.209 (12)
C22—C21	1.590 (8)	C25—C21	1.517 (10)
C26—C21	1.537 (12)	C27—C21	1.526 (9)
C23—C22	1.541 (8)	C30—C22	1.538 (11)
C31—C22	1.512 (11)	C24—C23	1.506 (12)
C32—C23	1.497 (8)	C25—C24	1.524 (9)
O28—C27	1.276 (10)	O29—C27	1.210 (10)
O33—C32	1.315 (9)	O34—C32	1.222 (9)
C5—C1—C2	105.2 (5)	C6—C1—C2	113.3 (6)
C6—C1—C5	110.6 (7)	C7—C1—C2	122.2 (6)
C7—C1—C5	109.8 (6)	C7—C1—C6	105.8 (5)
C3—C2—C1	99.7 (5)	C10—C2—C1	111.0 (6)
C10—C2—C3	110.0 (6)	C11—C2—C1	115.5 (6)
C11—C2—C3	113.8 (5)	C11—C2—C10	106.8 (7)
C4—C3—C2	105.1 (5)	C12—C3—C2	113.7 (7)
C12—C3—C4	114.0 (6)	C5—C4—C3	106.4 (6)
C4—C5—C1	107.6 (6)	O8—C7—C1	116.3 (6)
O9—C7—C1	122.6 (6)	O9—C7—O8	121.0 (6)
O13—C12—C3	117.2 (7)	O14—C12—C3	121.6 (7)
O14—C12—O13	121.2 (7)	C25—C21—C22	104.2 (5)
C26—C21—C22	110.0 (6)	C26—C21—C25	110.3 (7)
C27—C21—C22	110.4 (6)	C27—C21—C25	112.3 (6)
C27—C21—C26	109.6 (6)	C23—C22—C21	100.0 (5)
C30—C22—C21	109.8 (5)	C30—C22—C23	108.5 (5)
C31—C22—C21	114.4 (5)	C31—C22—C23	114.2 (5)
C31—C22—C30	109.5 (7)	C24—C23—C22	106.6 (5)
C32—C23—C22	113.4 (6)	C32—C23—C24	115.0 (6)
C25—C24—C23	107.3 (6)	C24—C25—C21	106.1 (6)
O28—C27—C21	115.0 (7)	O29—C27—C21	122.7 (6)
O29—C27—O28	122.3 (6)	O33—C32—C23	115.5 (6)
O34—C32—C23	122.7 (6)	O34—C32—O33	121.7 (6)
O8...O34 ⁱ	2.651 (4)	O13...O29 ⁱⁱ	2.652 (5)
O9...O33 ⁱ	2.608 (4)	O14...O28 ⁱⁱ	2.649 (5)

Symmetry codes: (i) $x - 1, y, z - 1$; (ii) $x, y, z - 1$.

Table 3. Atomic coordinates ($\times 10^4$) and equivalent isotropic thermal parameters ($\times 10^3$) for non-H atoms of (III)
$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	U_{eq} (\AA^2)
C1	7057 (6)	-2617 (7)	1471	37 (2)
C2	6316 (6)	-1983 (6)	782 (16)	37 (2)
C3	7373 (6)	-736 (6)	197 (16)	34 (2)
C4	8301 (8)	-969 (7)	-870 (17)	47 (2)
C5	8040 (7)	-2203 (8)	-161 (17)	46 (2)
C6	7588 (7)	-2244 (8)	3644 (18)	53 (3)
C7	6263 (7)	-3977 (7)	1498 (17)	41 (2)
O8	5379 (6)	-4368 (5)	2764 (15)	61 (2)
O9	6463 (5)	-4634 (5)	429 (15)	55 (2)
C10	5530 (7)	-2628 (7)	-1111 (18)	49 (3)
C11	5551 (8)	-1902 (8)	2476 (17)	51 (3)
C12	6986 (7)	-2 (7)	-1066 (18)	41 (2)
O13	6594 (5)	570 (5)	-83 (15)	44 (1)
O14	7033 (6)	-22 (6)	-3022 (15)	66 (2)
N15	6657 (6)	1285 (6)	-5929 (16)	46 (2)
O16	7209 (6)	2960 (5)	-687 (15)	68 (2)

and parallel to (20 $\bar{1}$). The two unique molecules of the asymmetric unit alternate along the chain. All bond lengths and angles have typical values, with

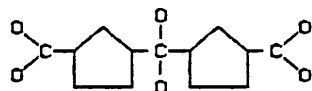
Table 4. *Interatomic distances (Å) and angles (°) and putative hydrogen-bond lengths (Å) for (III)*

C2—C1	1.611 (11)	C5—C1	1.518 (10)
C6—C1	1.506 (11)	C7—C1	1.539 (11)
C3—C2	1.558 (10)	C10—C2	1.525 (11)
C11—C2	1.502 (11)	C4—C3	1.540 (11)
C12—C3	1.513 (12)	C5—C4	1.533 (12)
O8—C7	1.281 (9)	O9—C7	1.217 (9)
O13—C12	1.258 (10)	O14—C12	1.239 (10)
C5—C1—C2	104.4 (6)	C6—C1—C2	112.2 (6)
C6—C1—C5	109.7 (7)	C7—C1—C2	111.2 (6)
C7—C1—C5	112.2 (7)	C7—C1—C6	107.2 (7)
C3—C2—C1	98.9 (5)	C10—C2—C1	109.8 (6)
C10—C2—C3	112.7 (6)	C11—C2—C1	115.5 (6)
C11—C2—C3	111.6 (6)	C11—C2—C10	108.2 (7)
C4—C3—C2	105.7 (6)	C12—C3—C2	112.5 (6)
C12—C3—C4	115.7 (6)	C5—C4—C3	107.0 (6)
C4—C5—C1	106.1 (7)	O8—C7—C1	114.6 (7)
O9—C7—C1	123.1 (7)	O9—C7—O8	122.3 (7)
O13—C12—C3	118.4 (8)	O14—C12—C3	118.6 (8)
O14—C12—O13	123.0 (8)		
O8 ⁱⁱⁱ ...O13	2.555 (9)	N15 ⁱⁱⁱ ...O13 ⁱⁱⁱ	2.775 (9)
O13 ⁱⁱⁱ ...O16	2.822 (10)	N15 ⁱⁱⁱ ...O14	2.710 (10)
O16 ⁱⁱⁱ ...O16 ⁱⁱⁱ	2.770 (9)	N15 ⁱⁱⁱ ...O16 ⁱⁱⁱ	2.891 (9)
N15 ⁱⁱⁱ ...O9 ⁱⁱⁱ	2.933 (9)	N15 ⁱⁱⁱ ...O9 ⁱⁱⁱ	3.165 (10)

Symmetry codes: (i) $-y, (x-y) - 1, (\frac{1}{3} + z) - 1$; (ii) $(y-x) + 2, 1-x, (\frac{1}{3} - z) - 1$; (iii) $x, y, 1+z$.

O8, O13, O28 and O33 carrying the acidic H atoms. The angles between the normals to the planes of the carboxylate groups and the plane C1, C3, C4, C5 of the appropriate five-membered ring are $40.4 (4)^\circ$ (C7), $32.8 (4)^\circ$ (C12), $37.4 (5)^\circ$ (C27) and $42.4 (4)^\circ$ (C32), respectively.

The model proposed for (II) contains folded chains not distinguishable from those in (I). However, in (II) the two unique molecules of the asymmetric unit form separate chains, parallel to **a**. One is quite normal, a sharply defined chain in which the molecules are, as in (I), successively 'up' or 'down' with respect to the median line of the chain. The second is clearly disordered. An electron density map shows the combination with an apparently



linear central O—C—O group. After many attempts, the best description allows the molecules of this second chain to adopt two positions relative to the first chain. These can be visualized as displacement by one molecule along the chain direction, so that a given position in the cell is occupied by either an 'up' or a 'down' molecule. Thus the combination shown above is interpreted as two 'up' molecules, one from each chain position and each with 50% site occupancy. Although this may not be a complete description of the disorder, the failure to obtain a satisfactory refinement probably reflects the inadequate data set as much as errors in the model.

(III) crystallizes in a trigonal space group. The threefold axis parallel to **c** through $x = 1/3, y = 2/3$ is surrounded by the C10 and C11 methyl groups, to give a non-polar region, whereas the threefold axis at $x = 2/3, y = 1/3$ is surrounded by firstly the water molecules, then the ammonium ions and finally the

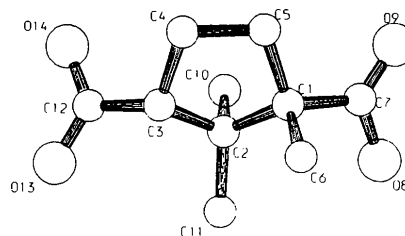


Fig. 1. Hydrogen camphorate anion in (III), showing numbering scheme common to (I) and (III).

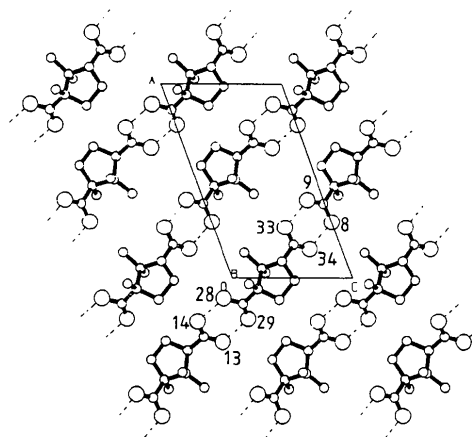


Fig. 2. Packing diagram for camphoric acid [form (I)] viewed down **b**, showing hydrogen-bond chains.

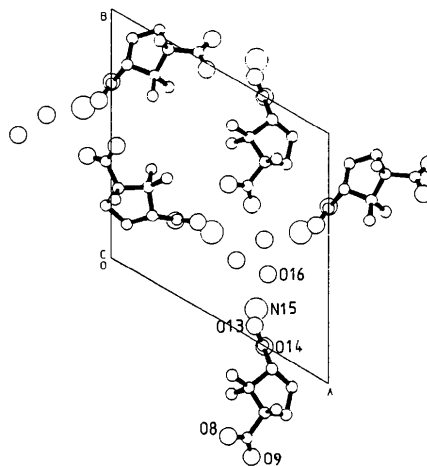


Fig. 3. Packing diagram for (III), viewed down **c**.

COOH and COO⁻ groups, Fig. 3. The bond lengths show clearly the difference between the acid group at C7 (O8 carries the hydrogen) and the anion at C12. The refinement showed more reasonable temperature parameters with the ammonium ion and the water molecule sited at N15 and O16 respectively than if these positions were reversed. Table 4 lists seven N...O and O...O contacts < 3.0 Å. Examination of angles and H-atom positions suggests that all of these are genuine hydrogen bonds, connecting the fragments into helices about the threefold axis. There are no other similar contacts < 3.3 Å. The angles between the normals to the planes of the carboxylate groups and the plane C1, C3, C4, C5 of the five-membered ring are 30.5 (5)° C(7) and 47.6 (6)° C(12).

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Structure and Conformation of 5-Bromo-2',3'-dideoxyuridine

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Abstract. C₉H₁₁BrN₂O₄, *M_r* = 291.11, monoclinic, *P*2₁, *a* = 11.307 (1), *b* = 5.954 (1), *c* = 15.829 (2) Å, β = 93.25 (1)°, *V* = 1063.90 Å³, *Z* = 4, *D_x* = 1.82 g cm⁻³, λ(Cu *Kα*) = 1.54184 Å, μ = 53.58 cm⁻¹, *F*(000) = 584, *T* = 295 K, *R* = 0.034 for 1927 observed reflections [*I* > 3σ(*I*)]. The crystal structure contains two independent molecules forming a dimer linked by a pair of N3—H...O2 hydrogen bonds; the crystal structure is stabilized by four additional hydrogen bonds. Two of these are internal C6—H6...O5' hydrogen bonds, one in molecule *A* and another in molecule *B*. These two molecules exhibit two different conformations; their sugar ring puckers are 2'-*endo*-3'-*exo* for molecule *A* and 3'-*endo*-2'-*exo* for molecule *B*. The C1'—N1 distance, the χ_{CN} torsion angle and the glycosidic conformation are 1.464 (8) Å, -130.0° and -anticlinal for molecule *A* and 1.506 (8) Å, -168.9° and -antiperiplanar for molecule *B*, respectively.

Introduction. Some selected modification of the chemical structure of nucleosides has produced anticancer, antiviral and antibacterial agents (Bloch, 1975; Prusoff, Cheng & Neenan, 1973; Hamor, O'Leary & Walker, 1978). The 5-substituted uracils

and the corresponding nucleosides have attracted attention because of their antiviral activity (Sharma & Bobek, 1975; Cheng, Domin, Sharma & Bobek, 1976). The crystal structure of 5-iodo-2'-deoxyuridine has been studied by Camerman & Trotter (1965). The 2',3'-dideoxy nucleoside derivatives have also been studied as potential antibiotics and antiviral agents (Atkinson, Deutcher, Kornberg, Russell & Moffatt, 1969; Chu, Schinazi, Ahn, Ullas & Gu, 1989). We are studying a series of 2',3'-dideoxy nucleosides in order to delineate the structure-function relationship of antiviral compounds (Parthasarathy & Kim, 1988). In this connection, we have studied the crystal structure of 5-bromo-2',3'-dideoxyuridine (BrddU); no study on the biological activity of this compound seems to have been carried out. However, this molecule also shows the same ranges of conformations (Parthasarathy & Kim, 1988; Van Roey, Salerno, Chu & Schinazi, 1989; Low, Tollin, Howie & Wilson, 1988) formed for AZT (3'-azido-3'-deoxythymidine) [several independent studies have been published on the crystal structure of AZT; the earliest one seems to be that of Gurskaya, Tsapkina, Skaptsova, Kracvskii, Lindeman & Struchkov (1986)] and other compounds which are active against HIV-1 in peripheral blood mononuclear cells.

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