Fig. 1. *ORTEP* drawing (Johnson, 1965) of the title compound with atom numbering. The anisotropic ellipsoids for non-H atoms enclose 30% probability.
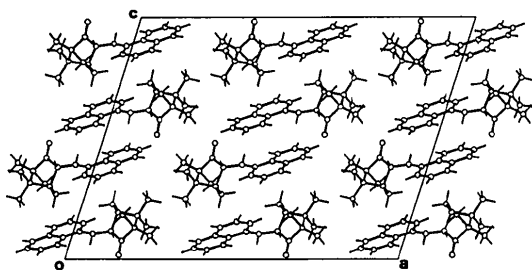

Fig. 2. A view of the unit cell.

2434 with $|F_o| > 3\sigma(|F_o|)$ used for structure determination, $2\theta_{max} = 125°$, *hkl* range: h −29 to 27, k 0–8, l 0–22, three standard reflections (02$\bar{9}$, 134 and 13,1,0) remeasured every 50 reflections without showing any significant change in intensity; corrections for Lorentz and polarization effects, absorption ignored; structure solved by direct methods with *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), refinement by full-matrix least squares on F

using *SHELX*76 (Sheldrick, 1976), all H atoms are on the difference map; anisotropic temperature factors for all non-H atoms and isotropic temperature factors for H atoms using riding model with C—H 1·00 Å for the 9-methyl group; $R = 0·050$, $wR = 0·068$, $w^{-1} = \sigma^2(F) + 0·00625F^2$, $S = 1·06$, $(\Delta/\sigma)_{max} = 0·03$, largest peak in final ΔF map 0·12 e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Table 1 contains final atomic coordinates and equivalent isotropic thermal parameters for non-H atoms.* Table 2 lists bond distances and angles. Fig. 1 shows the molecule and the numbering scheme adopted. Fig. 2 shows a view of the unit cell.

* Lists of anisotropic thermal parameters for non-H atoms, positional and thermal parameters for H atoms, bond distances and angles, and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51769 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of Cinnamamide

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Abstract. C_9H_9NO, $M_r = 147·08$, m.p. = 416–418 K, monoclinic, $P2_1/a$, $a = 16·015$ (3), $b = 5·072$ (1), $c = 9·563$ (2) Å, $\beta = 93·99$ (2)°, $V = 775·0$ (3) Å^3, $Z = 4$, $D_m = 1·26$ (2), $D_x = 1·261$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1·5418$ Å, $\mu = 0·63$ mm^{-1}, $F(000) = 312$, $T = 295$ K, $R = 0·066$ for 1042 reflections with $|F_o| > 2\sigma(F_o)$. The C=C double bonds of the nearest neighbours are related by $\bar{1}$ with a C$\cdots$C distance of 4·109 (4) Å, the interplanar spacing being 3·762 (4) Å for the planes through four C atoms involving the C=C bond. No topochemical reaction was observed.

Experimental. Crystals from a chloroform solution by slow evaporation. D_m by flotation in aqueous KI.

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Colourless prism elongated along **b**; 0·08 × 0·18 × 0·10 mm. Systematic absences h0l for h odd, 0k0 for k odd. Rigaku AFC-5 four-circle diffractometer equipped with rotating anode (40 kV, 200 mA), Ni-filtered Cu $K\alpha$. 20 reflections within $14 < 2\theta < 38°$ used to determine the lattice parameters. Intensity data collected within $2\theta_{max} = 125°$ ($-18 \leq h \leq 18$, $0 \leq k \leq 5$, $0 \leq l \leq 11$), $\omega-2\theta$ scan method [scan speed 4° min^{-1} in ω, scan range $(1·2 + 0·15\tan\theta)°$ in ω], background measured for 4 s on either side of the peak, three standard reflections recorded after every 57 reflections, fluctuations within 1%. Lorentz and polarization corrections, no absorption correction. 1235 unique reflections measured, $R_{int} = 0·022$ for 79 hk0 reflections. 1042 reflections with $|F_o| > 2\sigma(F_o)$ used in the structure analysis. Structure solved by Patterson method and refined by block-diagonal least squares (non-H atoms anisotropically). H atoms determined from a difference Fourier map and refined isotropically; $\sum w(|F_o| - |F_c|)^2$ minimized with $w = 1·0/[\sigma(F_o)^2 + 0·0269|F_o| + 0·0003|F_o|^2]$. Correction for secondary extinction applied for six strongest reflections [$I_{corr} = I_o(1 + 2·4 \times 10^{-5}I_o)$]. Final $R = 0·066$ for 1042 reflections, $wR = 0·089$, $S = 1·26$, $(\Delta/\sigma)_{max} = 0·2$. The residual electron density in the final difference map was within ±0·27 e Å^{-3}. No change was observed for crystals exposed to sunlight for two months.

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Programs: *RSSFR-5* (Sakurai, 1967), *HBLS*-V and *DAPH* (Ashida, 1973), *MOLCON* (Fujii, 1979) and *ORTEP*II (Johnson, 1971). Computations carried out at the Crystallographic Research Center, Institute for Protein Research, Osaka University, and at the Okayama University Computer Center. The final atomic parameters are listed in Table 1.* The thermal ellipsoids of the molecule are shown in Fig. 1 with atomic numbering. Bond lengths and angles are listed in Table 2. A stereoscopic view of the crystal structure is shown in Fig. 2.

Related literature. The lattice parameters, space group and two-dimensional structure of the title compound have been described by Schmidt (1964). However, no three-dimensional structure has been published. We have determined the structure as part of studies of solid-state photoreactions (Kashino, Oka & Haisa, 1989; Iwamoto, Kashino & Haisa, 1989). In the crystals the molecules are held together by N—H···O hydrogen bonds between the amide groups as in

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, and bond lengths and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51797 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final atomic coordinates (× 10^4) and equivalent isotropic thermal parameters (Å^2) with e.s.d.'s in parentheses*

$$B_{eq} = (4/3)\sum_i\beta_{ii}/a_{ii}^{*2}.$$

	x	y	z	B_{eq}
O(1)	4571 (2)	−2029 (4)	8475 (2)	5·1 (1)
N(1)	4377 (2)	2282 (5)	8871 (3)	4·3 (1)
C(1)	3633 (2)	−1222 (6)	4191 (3)	4·6 (1)
C(2)	3039 (2)	619 (7)	3719 (3)	4·4 (1)
C(3)	2709 (2)	602 (8)	2348 (4)	5·2 (2)
C(4)	2977 (2)	−1251 (8)	1424 (3)	5·7 (2)
C(5)	3554 (2)	−3078 (9)	1873 (4)	5·9 (2)
C(6)	3881 (2)	−3101 (8)	3255 (4)	5·1 (2)
C(7)	3992 (2)	−1300 (6)	5639 (3)	4·0 (1)
C(8)	3931 (2)	535 (6)	6621 (3)	4·1 (1)
C(9)	4323 (2)	163 (6)	8061 (3)	3·8 (1)

Table 2. *Bond lengths (Å) and angles (°) with e.s.d.'s in parentheses*

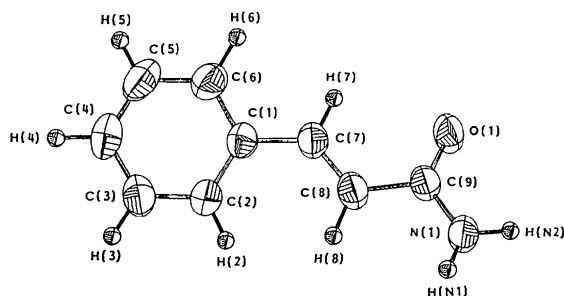|			
O(1)–C(9)	1·236 (4)	C(3)–C(4)	1·379 (6)
N(1)–C(9)	1·324 (4)	C(4)–C(5)	1·357 (6)
C(1)–C(2)	1·386 (5)	C(5)–C(6)	1·387 (6)
C(1)–C(6)	1·384 (5)	C(7)–C(8)	1·331 (4)
C(1)–C(7)	1·462 (4)	C(8)–C(9)	1·485 (4)
C(2)–C(3)	1·379 (6)		
O(1)–C(9)–N(1)	122·4 (3)	C(2)–C(1)–C(6)	118·3 (3)
O(1)–C(9)–C(8)	121·1 (3)	C(2)–C(1)–C(7)	122·8 (3)
N(1)–C(9)–C(8)	116·5 (3)	C(3)–C(4)–C(5)	119·9 (4)
C(1)–C(2)–C(3)	121·0 (4)	C(4)–C(5)–C(6)	120·7 (4)
C(1)–C(6)–C(5)	120·3 (4)	C(6)–C(1)–C(7)	118·8 (3)
C(1)–C(7)–C(8)	127·3 (3)	C(7)–C(8)–C(9)	121·2 (3)
C(2)–C(3)–C(4)	119·9 (4)		

Fig. 1. The thermal ellipsoids of the molecule with atomic numbering. Ellipsoids of 50% probability are drawn for the non-H atoms; the H atoms are represented as spheres equivalent to $B = 1·0$ Å^2.
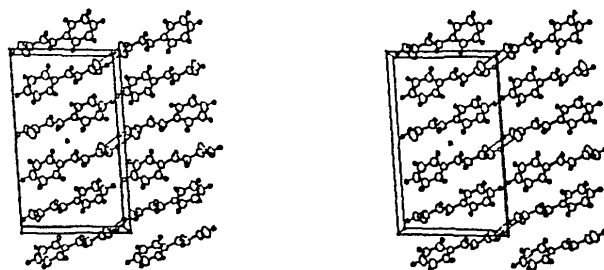

Fig. 2. Stereoscopic view of the crystal structure. The a axis points upwards, the b axis onto the plane of the paper and the c axis left to right.

benzamide (Blake & Small, 1972): (a) N(1)—H(N2)···
O(1)(1−x, −y, 2−z) [N···O 2·950 (4), H···O
2·02 (3) Å, N—H···O 170 (3)°]; (b) N(1)—H(N1)···
O(1)(x, 1+y, z) [N···O 2·930 (4), H···O 2·09 (3) Å,
N—H···O 160 (1)°].

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Structure of 6-Amino-1,6-dideoxy-1-[3,4-dihydro-3-methyl-2,4-dioxo-1(2H)-pyrimidinyl]-4-thio-L-glycero-α-L-ido-heptofuranuronic Acid Monohydrate

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Abstract. $C_{12}H_{17}N_3O_7S.H_2O$, $M_r = 365·36$, mono-
clinic, $P2_1$, $a = 15·105$ (2), $b = 7·915$ (1), $c =$
6·451 (1) Å, $\beta = 91·29$ (1)°, $V = 771·1$ Å^3, $Z = 2$,
$D_x = 1·574$ g cm^{-3}, $\lambda(Cu K\alpha) = 1·5418$ Å, $\mu =$
22·806 cm^{-1}, $F(000) = 384$, $T = 298$ K, final $R =$
0·062 for 1665 unique reflections $[F_o^2 > 2\sigma(F_o^2)]$. The
thiofuranosyl ring adopts an envelope conformation
(E_3). The pyrimidyl moiety of the title compound is in a
+anti orientation $(\chi = -133·5°)$, in contrast to the
methyl ester of the tetraacetylsulfoxide derivative which
adopts a +syn orientation $(\chi = 67·7°)$.

Experimental. Colorless prisms of title compound were
grown from an aqueous ethanol solution [H$_2$O/

$C_2H_5OH = 1 : 1$ (v/v)] at 277 K. Crystal size 0·38 ×
0·20 × 0·18 mm, Enraf–Nonius CAD-4 diffractom-
eter, Cu Kα radiation, graphite monochromator, θ–2θ

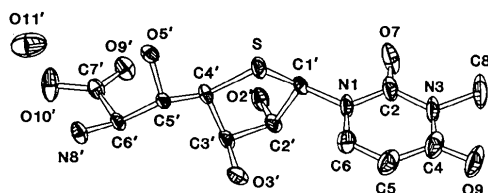* To whom correspondence should be addressed.

Fig. 1. Perspective view of the molecule with the numbering scheme.
To show the absolute configuration correctly, the figure was
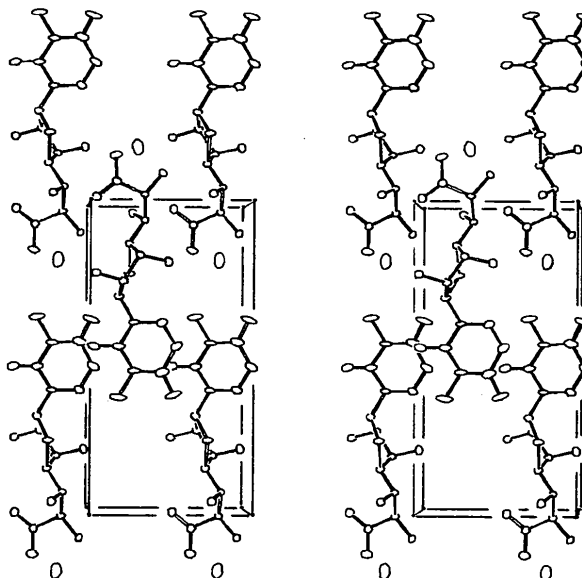drawn in the left-handed coordinate system.

Fig. 2. Stereoscopic view of the crystal packing. The projection is
down [001] and the b axis is horizontal.