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Crystal Structure of 3-*O*-Acetyl-1,2-*O*-isopropylidene-5-*O*-tosyl-α-D-gulofuranose-4,6-carbolactone

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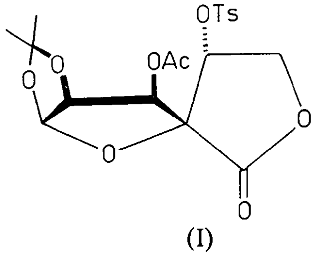
Crystals of 3-*O*-acetyl-1,2-*O*-isopropylidene-5-*O*-tosyl-α-D-gulofuranose-4,6-carbolactone are orthorhombic, space group $P2_12_12_1$, with $a = 9{\cdot}782$, $b = 10{\cdot}455$, $c = 19{\cdot}976$ Å and $Z = 4$. The structure was solved by direct methods and refined by full-matrix least squares to $R = 0{\cdot}041$. Bond lengths and angles are close to normal values.

Introduction

Photoamidation of 3-*O*-acetyl-1,2:5,6-di-*O*-isopropylidene-α-D-*erythro*-hex-3-enofuranose afforded two products in 65 and 26% yields. Treatment of the major product with 5% hydrochloric acid, followed by tosylation, gave 3-*O*-acetyl-1,2-*O*-isopropylidene-5-*O*-tosyl-α-D-gulofuranose-4,6-carbolactone (I) (Rosenthal & Ratcliffe, 1976).



(I)

The crystal structure of (I) was studied in order to determine the configurations at C(3) and C(4).

Experimental

A small piece (dimensions *ca* 0·040 × 0·024 × 0·012 cm) was cut from a large needle and used for data collection. Unit-cell and intensity data were measured on a Datex-automated GE XRD 6 diffractometer with Cu $K\alpha$ radiation and the θ–2θ scan technique. Unit-cell parameters were refined by least squares from the observed 2θ values of 15 reflexions.

Crystal data

$C_{19}H_{22}O_{10}S$, FW 442·44; $a = 9{\cdot}782\,(2)$, $b = 10{\cdot}455\,(4)$, $c = 19{\cdot}976\,(6)$ Å; $V = 2043\,(1)$ Å^3, $d_m = 1{\cdot}42$ (flotation), $d_x = 1{\cdot}438$ g cm^{-3}, $Z = 4$. Space group $P2_12_12_1$ ($h00$, $h = 2n$; $0k0$, $k = 2n$; $00l$, $l = 2n$). Cu $K\alpha$ radiation, Ni-filtered; $\lambda(\text{Cu } K\alpha) = 1{\cdot}5418$ Å, $\mu(\text{Cu } K\alpha) = 18{\cdot}7$ cm^{-1}.

Of the 2331 independent reflexions with $2\theta < 146°$, 2016 had intensities greater than $3\sigma(I)$ above background [$\sigma^2(I) = S + B + (0{\cdot}05S)^2$, where S = scan and B = background count]. Lorentz and polarization corrections were applied and the structure amplitudes derived. No absorption correction was applied.

Structure determination and refinement

The structure was solved by direct methods with symbolic addition and tangent-refinement techniques. Origin-defining reflexions and starting symbols were chosen manually. The set of phases with the highest consistency gave an E map showing the S and seventeen other non-hydrogen atoms. One cycle of full-matrix least-squares refinement was carried out where the function minimized was $\Sigma\ w(|F_o| - |F_c|)^2$, with weights $w = 1{\cdot}0$. A difference Fourier map then revealed the remaining non-hydrogen atoms. Refinement was continued with weights $w = 1/\sigma^2(F)$ [$\sigma(F)$ values were derived from the previously calculated $\sigma(I)$ values] and anisotropic temperature factors. All H atoms were located on a difference map and included in the refinement with isotropic temperature factors.

The final R and R' $\{=[\Sigma\ w(|F_o| - |F_c|)^2/\Sigma\ w|F_o|^2]^{1/2}\}$ for the 2016 reflexions with $I > 3\sigma(I)$ are 0·041 and

Table 1. *Final positional parameters (fractional*, × 10^4, S × 10^5, H × 10^3) *with estimated standard deviations in parentheses*

	x	*y*	*z*
S	−30988 (9)	8928 (10)	12243 (5)
O(51)	−2864 (2)	2017 (2)	1739 (1)
C(5)	−3767 (4)	2118 (4)	2316 (2)
C(6)	−5079 (4)	2815 (4)	2113 (2)
O(61′)	−4710 (3)	4165 (3)	2121 (1)
C(1′)	−3631 (4)	4358 (4)	2517 (2)
C(4)	−3085 (4)	3085 (3)	2783 (2)
C(3)	−3433 (4)	2886 (4)	3530 (2)
C(2)	−2254 (4)	2087 (4)	3787 (2)
C(1)	−1092 (4)	2395 (4)	3296 (2)
O(41)	−1653 (3)	3127 (3)	2770 (1)
O(1)	−644 (3)	1215 (3)	3063 (2)
C(11)	−1230 (4)	213 (4)	3460 (2)
O(2)	−2488 (3)	761 (3)	3686 (1)
C(12)	−1536 (6)	−905 (6)	3010 (3)
C(13)	−301 (6)	−128 (7)	4030 (3)
O(1′)	−3199 (4)	5407 (3)	2634 (2)
O(31)	−4760 (3)	2313 (3)	3581 (1)
C(32)	−5412 (5)	2435 (4)	4175 (2)
C(33)	−6843 (7)	1973 (7)	4113 (4)
O(34)	−4875 (5)	2878 (4)	4654 (2)
O(52)	−3454 (3)	−221 (3)	1590 (2)
O(53)	−4015 (3)	1310 (4)	713 (2)
C(54)	−1433 (3)	814 (4)	902 (2)
C(55)	−323 (4)	860 (5)	1336 (2)
C(56)	974 (4)	865 (5)	1063 (2)
C(57)	1193 (4)	835 (4)	378 (2)
C(58)	60 (4)	742 (5)	−33 (2)
C(59)	−1260 (4)	741 (5)	222 (2)
C(60)	2627 (5)	912 (7)	115 (4)
H(5)	−395 (4)	132 (4)	249 (2)
H(6*a*)	−536 (5)	261 (4)	162 (2)
H(6*b*)	−582 (6)	275 (5)	242 (2)
H(3)	−346 (5)	364 (5)	377 (2)
H(2)	−206 (4)	224 (4)	426 (2)
H(1)	−34 (5)	281 (5)	347 (2)
H(12*a*)	−199 (8)	−131 (7)	343 (4)
H(12*b*)	−70 (9)	−133 (8)	281 (4)
H(12*c*)	−205 (6)	−53 (5)	264 (3)
H(13*a*)	−76 (5)	−92 (5)	428 (3)
H(13*b*)	41 (6)	−42 (6)	385 (3)
H(13*c*)	−4 (7)	79 (7)	422 (4)
H(33*a*)	−714 (12)	176 (10)	371 (5)
H(33*b*)	−711 (10)	173 (9)	462 (5)
H(33*c*)	−738 (15)	258 (15)	407 (9)
H(55)	−50 (5)	84 (5)	187 (2)
H(56)	161 (9)	100 (8)	138 (4)
H(58)	27 (5)	68 (5)	−50 (3)
H(59)	−205 (5)	74 (4)	−9 (2)
H(60*a*)	259 (6)	114 (6)	−34 (3)
H(60*b*)	337 (9)	181 (8)	31 (4)
H(60*c*)	287 (6)	−1 (6)	11 (2)

Table 2. *Final thermal parameters and their estimated standard deviations*

(*a*) Anisotropic thermal parameters (U_{ij} × 10^3, S × 10^4 Å²) in the expression:

$$f = f^0 \exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)].$$

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S	405 (4)	590 (6)	431 (4)	−41 (4)	26 (4)	−112 (4)
O(51)	42 (1)	43 (1)	48 (1)	−5 (1)	11 (1)	−6 (1)
C(5)	37 (2)	43 (2)	45 (2)	1 (2)	7 (1)	−2 (2)
C(6)	38 (2)	49 (2)	54 (2)	1 (2)	−2 (2)	−8 (2)
O(61′)	50 (1)	46 (1)	70 (2)	11 (1)	−4 (1)	5 (2)
C(1′)	49 (2)	47 (2)	58 (2)	1 (2)	4 (2)	−2 (2)
C(4)	39 (2)	38 (2)	48 (2)	0 (2)	3 (2)	−1 (1)
C(3)	50 (2)	48 (2)	45 (2)	2 (2)	4 (2)	−13 (2)
C(2)	52 (2)	61 (2)	44 (2)	7 (2)	−2 (2)	−7 (2)
C(1)	40 (2)	54 (2)	57 (2)	−3 (2)	−9 (2)	−4 (2)
O(41)	38 (1)	56 (1)	57 (1)	−3 (1)	−1 (1)	1 (1)
O(1)	60 (2)	52 (2)	70 (2)	8 (1)	20 (1)	6 (1)
C(11)	41 (2)	55 (2)	51 (2)	3 (2)	−1 (2)	8 (2)
O(2)	42 (1)	59 (2)	68 (2)	9 (1)	8 (1)	13 (2)
C(12)	64 (3)	68 (3)	82 (3)	15 (3)	−21 (3)	0 (3)
C(13)	61 (3)	94 (4)	65 (3)	23 (3)	−12 (2)	9 (3)
O(1′)	80 (2)	42 (1)	101 (2)	−2 (2)	−13 (2)	−1 (2)
O(31)	43 (1)	50 (1)	50 (1)	2 (1)	8 (1)	−5 (1)
C(32)	71 (3)	54 (3)	59 (3)	9 (2)	21 (2)	4 (2)
C(33)	72 (3)	84 (4)	92 (4)	−3 (3)	36 (3)	11 (3)
O(34)	116 (3)	104 (3)	54 (2)	−11 (3)	22 (2)	−14 (2)
O(52)	75 (2)	52 (2)	69 (2)	−23 (2)	18 (2)	−10 (1)
O(53)	48 (2)	118 (3)	57 (2)	14 (2)	−10 (1)	−12 (2)
C(54)	44 (2)	45 (2)	42 (2)	6 (2)	2 (1)	−3 (2)
C(55)	46 (2)	66 (2)	46 (2)	5 (2)	−3 (2)	−5 (2)
C(56)	42 (2)	57 (2)	67 (2)	6 (2)	−5 (2)	−13 (2)
C(57)	47 (2)	49 (2)	73 (2)	7 (2)	13 (2)	−6 (2)
C(58)	58 (2)	79 (3)	49 (2)	17 (2)	14 (2)	−2 (2)
C(59)	51 (2)	68 (3)	43 (2)	7 (2)	3 (2)	−3 (2)
C(60)	57 (3)	89 (4)	98 (4)	13 (3)	27 (3)	−5 (4)

(*b*) Isotropic thermal parameters (U × 10^2)

	U (Å²)		*U* (Å²)		*U* (Å²)
H(5)	4 (1)	H(6*a*)	6 (1)	H(6*b*)	7 (2)
H(3)	6 (1)	H(2)	5 (1)	H(1)	7 (1)
H(12*a*)	13 (2)	H(12*b*)	13 (3)	H(12*c*)	10 (2)
H(13*a*)	7 (1)	H(13*b*)	10 (2)	H(13*c*)	12 (2)
H(33*a*)	17 (4)	H(33*b*)	16 (3)	H(33*c*)	34 (8)
H(55)	6 (1)	H(56)	11 (3)	H(58)	8 (1)
H(59)	7 (1)	H(60*a*)	11 (2)	H(60*b*)	15 (3)
H(60*c*)	9 (2)				

0·055 respectively (0·048 and 0·063 for the other enantiomer). For all 2331 data R is 0·049 and R' is 0·055.* The correct absolute configuration has been determined, from comparison of the R values for the two enantiomorphs (Hamilton, 1965), to be that shown in Fig. 1 with better than 99·5% significance. The enantiomer is as predicted from the chemical preparation. The error in an observation of unit weight $\{[\Sigma\, w(|F_o| - |F_c|)^2/(m-n)]^{1/2}\}$ is 1·57.

Atomic scattering factors for S, O and C atoms are those of Cromer & Mann (1968) and for H atoms those of Stewart, Davidson & Simpson (1965). The real and imaginary parts of the anomalous scattering factors for S, O and C atoms were taken from Cromer & Liberman (1970). Final positional and thermal parameters are listed in Tables 1 and 2.

Thermal-motion analysis

Thermal-motion analysis and correction of bond lengths for libration were carried out with methods previously described (Phillips & Trotter, 1976). The molecule was divided into five segments (each forming a good rigid body) as follows: (1) the phenyl ring, (2) the tetrahedral O_3SC group, (3) the two spiro-fused five-membered rings, (4) the *O*-acetyl group, and (5) the $(Me)_2CO_2$ isopropylidene group. Corrected bond lengths are given in Table 3. The effects of the correction are reflected in the weighted mean C—C bond length in the phenyl ring, which increased from 1·383 (3) to 1·392 (3) Å. Bond angles are not significantly affected and uncorrected values only are given in Table 4.

Table 4. *Bond angles (°) with estimated standard deviations in parentheses for non-hydrogen atoms*

O(51)—S—O(52)	108·1 (2)	O(51)—S—O(53)	109·3 (2)
O(51)—S—C(54)	98·0 (2)	O(52)—S—O(53)	117·8 (2)
O(52)—S—C(54)	112·2 (2)	O(53)—S—C(54)	109·6 (2)
S—O(51)—C(5)	118·8 (2)	O(51)—C(5)—C(6)	109·5 (3)
O(51)—C(5)—C(4)	105·5 (3)	C(4)—C(5)—C(6)	102·3 (3)
C(5)—C(6)—O(61′)	104·5 (3)	C(6)—O(61′)—C(1′)	110·5 (3)
O(1′)—C(1′)—O(61′)	122·4 (3)	O(1′)—C(1′)—C(4)	127·2 (4)
O(61′)—C(1′)—C(4)	110·5 (3)	C(5)—C(4)—C(1′)	102·2 (3)
C(5)—C(4)—O(41)	116·5 (3)	C(5)—C(4)—C(3)	113·8 (3)
C(1′)—C(4)—O(41)	108·4 (3)	C(1′)—C(4)—C(3)	112·1 (3)
O(41)—C(4)—C(3)	104·0 (3)	C(4)—C(3)—C(2)	103·5 (3)
C(4)—C(3)—O(31)	109·9 (3)	C(2)—C(3)—O(31)	115·9 (3)
C(3)—C(2)—C(1)	103·4 (3)	C(3)—C(2)—O(2)	111·6 (3)
C(1)—C(2)—O(2)	103·5 (3)	C(2)—C(1)—O(41)	107·6 (3)
C(2)—C(1)—O(1)	105·1 (3)	O(41)—C(1)—O(1)	110·8 (3)
C(1)—O(41)—C(4)	111·0 (3)	C(1)—O(1)—C(11)	109·7 (3)
C(2)—O(2)—C(11)	107·3 (3)	O(1)—C(11)—O(2)	103·1 (3)
O(1)—C(11)—C(12)	108·5 (4)	O(1)—C(11)—C(13)	110·5 (4)
O(2)—C(11)—C(12)	109·2 (3)	O(2)—C(11)—C(13)	112·1 (4)
C(12)—C(11)—C(13)	112·9 (4)	C(3)—O(31)—C(32)	116·7 (3)
O(31)—C(32)—C(33)	109·8 (5)	O(31)—C(32)—O(34)	122·4 (4)
C(33)—C(32)—O(34)	127·7 (5)	S—C(54)—C(55)	119·6 (3)
S—C(54)—C(59)	118·8 (3)	C(55)—C(54)—C(59)	121·6 (3)
C(54)—C(55)—C(56)	118·1 (3)	C(55)—C(56)—C(57)	122·1 (4)
C(56)—C(57)—C(58)	117·6 (4)	C(56)—C(57)—C(60)	119·3 (4)
C(58)—C(57)—C(60)	123·1 (4)	C(57)—C(58)—C(59)	121·9 (4)
C(54)—C(59)—C(58)	118·6 (4)		

Results and discussion

A stereo diagram of the molecule (Fig. 1) shows the absolute configuration and the crystallographic number-

Table 3. *Bond lengths (Å) with estimated standard deviations in parentheses for non-hydrogen atoms*

	Uncorrected	Corrected		Uncorrected	Corrected
S—O(51)	1·579 (3)	1·589	S—O(52)	1·418 (3)	1·429
S—O(53)	1·427 (3)	1·439	S—C(54)	1·754 (3)	1·763
O(51)—C(5)	1·455 (4)	1·457	C(5)—C(6)	1·531 (5)	1·534
C(5)—C(4)	1·529 (5)	1·532	C(6)—O(61′)	1·457 (5)	1·459
C(61′)—C(1′)	1·333 (5)	1·336	C(1′)—O(1′)	1·198 (5)	1·201
C(1′)—C(4)	1·530 (5)	1·533	C(4)—C(3)	1·546 (5)	1·550
C(4)—O(41)	1·402 (4)	1·405	C(3)—O(31)	1·433 (5)	1·436
C(3)—C(2)	1·513 (6)	1·516	C(2)—C(1)	1·536 (6)	1·538
C(2)—O(2)	1·420 (5)	1·430	O(41)—C(1)	1·411 (5)	1·414
C(1)—O(1)	1·390 (5)	1·394	O(1)—C(11)	1·433 (5)	1·446
C(11)—C(12)	1·505 (7)	1·518	C(11)—C(13)	1·500 (6)	1·514
C(11)—O(2)	1·431 (5)	1·439	O(31)—C(32)	1·355 (5)	1·377
C(32)—C(33)	1·486 (8)	1·493	C(32)—O(34)	1·185 (6)	1·197
C(54)—C(55)	1·391 (5)	1·400	C(54)—C(59)	1·372 (5)	1·384
C(55)—C(56)	1·382 (6)	1·386	C(56)—C(57)	1·386 (6)	1·398
C(57)—C(58)	1·383 (6)	1·391	C(57)—C(60)	1·500 (6)	1·503
C(58)—C(59)	1·387 (6)	1·391			

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32155 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

ing scheme. Bonds and angles in the tosyl group are normal and agree well with previously reported values (McConnell, Angyal & Stevens, 1972), except that the S=O bonds differ in length by 3σ. The phenyl ring is slightly, but significantly, non-planar with the S atom lying 0·10 Å from the mean plane.

The five-membered ring containing C(5) has the envelope conformation, C(5) lying 0·49 Å from the mean plane through the other four atoms. Bond lengths in the ring are normal, except for the very short O(61′)—C(1′) distance, 1·336 Å. The other CCCCO ring has slightly twisted envelope conformation, C(4) lying 0·45 Å from the four-atom mean plane.

The CCOCO ring has a similar twisted envelope conformation, C(11) lying 0·46 Å from the four-atom mean plane. Rings of this type are quite flexible and are found with a range of conformations (Willy, Binsch & Eliel, 1970). Bond lengths and angles in the ring agree with previously reported values (Riche & Pascard-Billy, 1975), C(1)—O(1) being a little short. The short C(11)—C(12) and C(11)—C(13) bonds are normal for *O*-isopropylidene groups. The *O*-acetyl group is planar

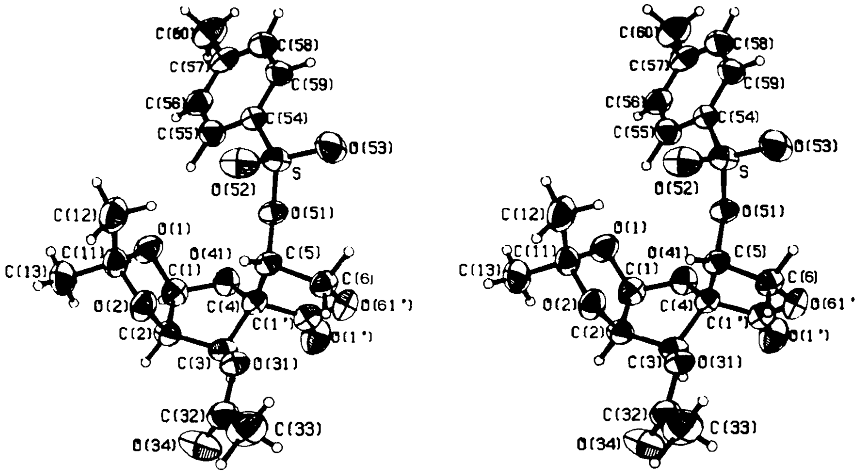

Fig. 1. Stereo diagram of 3-*O*-acetyl-1,2-*O*-isopropylidene-5-*O*-tosyl-α-D-gulofuranose-4,6-carbolactone with 50% vibration ellipsoids for non-hydrogen atoms.

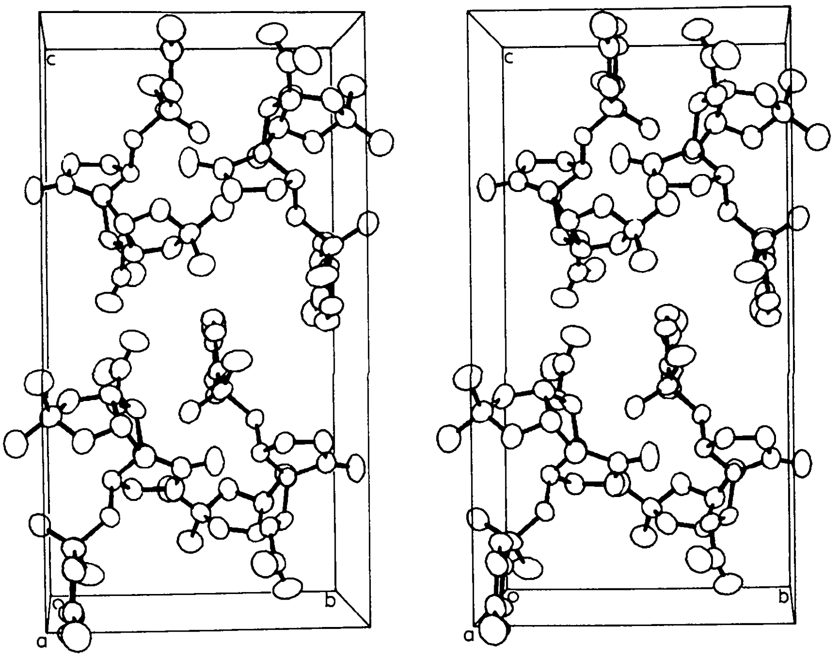

Fig. 2. An *a* projection of the structure.

within experimental error, its mean plane making an angle of 58·6° with the four-atom plane of the neighbouring ring.

Non-bonded distances correspond to van der Waals contacts with a few exceptions. H(55) · · · O(1) is 2·42 Å, suggesting a C—H · · · O interaction, with an angle of 168° subtended at the H. This is probably responsible for holding the tosyl group in the conformation observed. A similar, but weaker, intermolecular interaction occurs between O(1′) and H(56)$[-x, \frac{1}{2} + y, \frac{1}{2} - z]$. O · · · H is 2·58 Å and the angle at H is 156°. The packing arrangement in the unit cell is shown in Fig. 2.

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The Crystal Structure of 1-Phenyl-4,5-dihydro-7,8-dihydroxy-1*H*-benz[*g*]indazole, $C_{17}H_{14}N_2O_2$

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The crystal structure of 1-phenyl-4,5-dihydro-7,8-dihydroxy-1*H*-benz[*g*]indazole, $C_{17}H_{14}N_2O_2$, has been determined and refined by least-squares methods. The crystals are triclinic, space group $P\bar{1}$, $Z = 4$ with $a =$ 10·9774 (7), $b =$ 11·1683 (8), $c =$ 14·2764 (8) Å, $\alpha =$ 92·164 (5), $\beta =$ 121·613 (4), $\gamma =$ 109·132 (6)°. The final R value is 0·056 for the 5166 reflections used in the structure determination. The two independent molecules are linked in parallel chains by two strong hydrogen bonds, O(14) · · · N(23) (2·719 Å) and O(35) · · · N(2) (2·728 Å), approximately in the $[0\bar{1}1]$ direction.

Introduction

The title compound is a highly substituted pyrazole, synthesized for potential use in cancer chemotherapy (Hashem, Berlin, Chesnut & Durham, 1976). It inhibits the growth of *Bacillus subtilis* at 91 μg ml^{-1} and reduces KB cell proliferation by 50% at a concentration less than 25 μg ml^{-1}. The present compound is from a group of five for which we hope to obtain structure–activity relations.

Experimental

A single crystal of parallelepiped shape with the dimensions 0·14 × 0·18 × 0·22 mm, obtained from a slow evaporation of a 95% ethanol solution at room temperature, was chosen for the data collection. The space group was determined as triclinic. The least-squares cell dimensions were determined with Cu $K\alpha_1$ radiation (λ = 1·5405 Å) from the 2θ values of 44 reflections spaced throughout reciprocal space. The crystal data