

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
F	4521 (3)	2126 (4)	809 (1)	45 (1)
N(1)	11117 (4)	567 (4)	-595 (1)	28 (1)
N(2)	10399 (4)	2215 (4)	-174 (1)	28 (1)
C(3)	9297 (5)	1603 (5)	409 (2)	24 (1)
N(4)	8614 (4)	3329 (5)	838 (1)	30 (1)
C(5)	7551 (5)	2924 (6)	1505 (2)	27 (1)
C(6)	5281 (5)	3252 (5)	1384 (2)	28 (1)
N(7)	4050 (4)	2507 (5)	2052 (2)	36 (1)
O(7a)	4971 (4)	2489 (5)	2642 (1)	52 (1)
O(7b)	2320 (5)	1988 (8)	1937 (2)	80 (1)
N(8)	4744 (4)	5802 (5)	1280 (2)	36 (1)
O(8a)	5444 (4)	7108 (4)	1744 (1)	48 (1)
O(8b)	3707 (6)	6309 (6)	750 (2)	83 (1)

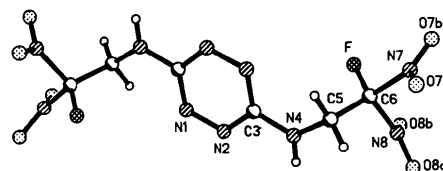


Fig. 1. Perspective drawing of the results of the X-ray study on the diaminotetrazine.

Related literature. The structures of other compounds containing nitro groups and F atoms have been reported (Koppes, Chaykovsky, Adolph, Gilardi & George, 1987). In 1,4-difluoro-1,1,4,4-tetranitro-2,3-butanediyl diacetate (Flippen-Anderson, George & Gilardi, 1988) the fluoro nitro moiety displayed a geometry similar to that found for this molecule.

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Table 2. Bond lengths (\AA) and bond angles ($^\circ$)

F—C(6)	1.321 (4)	N(1)—N(2)	1.320 (3)
N(2)—C(3)	1.346 (4)	C(3)—N(4)	1.354 (4)
C(3)—N(1')	1.337 (4)	N(4)—C(5)	1.432 (4)
C(5)—C(6)	1.514 (5)	C(6)—N(7)	1.536 (4)
C(6)—N(8)	1.537 (4)	N(7)—O(7a)	1.217 (4)
N(7)—O(7b)	1.190 (4)	N(8)—O(8a)	1.217 (4)
N(8)—O(8b)	1.203 (4)		
C(3)—N(2)—N(1)	118.0 (2)	N(4)—C(3)—N(2)	116.6 (3)
N(4)—C(3)—N(1')	119.0 (3)	N(2)—C(3)—N(1')	124.4 (3)
C(5)—N(4)—C(3)	122.6 (3)	C(6)—C(5)—N(4)	110.8 (2)
C(5)—C(6)—F	113.9 (3)	N(7)—C(6)—F	106.7 (2)
N(7)—C(6)—C(5)	112.7 (2)	N(8)—C(6)—F	107.5 (2)
N(8)—C(6)—C(5)	111.2 (3)	N(8)—C(6)—N(7)	104.2 (2)
O(7a)—N(7)—C(6)	115.9 (3)	O(7b)—N(7)—C(6)	116.9 (3)
O(7b)—N(7)—O(7a)	127.1 (3)	O(8a)—N(8)—C(6)	115.9 (3)
O(8b)—N(8)—C(6)	117.3 (3)	O(8b)—N(8)—O(8a)	126.7 (3)

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Structure of 1,2-*O*-Isopropylidene- α -D-allofuranose

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Abstract. $C_9H_{16}O_6$, $M_r = 220.2$, orthorhombic, $P2_12_12_1$, $a = 6.075$ (2), $b = 6.776$ (2), $c = 25.975$ (7) \AA , $V = 1069.2$ \AA^3 , $Z = 4$, $D_x = 1.368$ Mg m^{-3} , $\lambda(\text{Cu } K\alpha) = 1.5418$ \AA , $\mu = 0.89$ mm^{-1} , $F(000) = 472$, $T = 293$ K, $R = 0.028$ for 932 unique observed reflections [$F > 3\sigma(F)$]. The fused five-membered rings both have envelope conformations with maximum distances from the best least-squares plane for each ring of 0.159 (3) \AA for C2 and 0.209 (2) \AA for C3 and an angle between the planes of 109.8 (6) $^\circ$. The three hydroxyl groups form hydrogen bonds which make a spiral arrangement parallel to the a axis:

O(3)—HO3...O5, O5—HO5...O6 and O6—HO6...O3 with O—O distances of 3.045, 2.699 and 2.827 \AA respectively.

Experimental. The commercial sample was recrystallized from a mixture of acetone and petroleum ether. Crystal tabular, 0.50 \times 0.17 \times 0.09 mm, Enraf-Nonius CAD-4F diffractometer, Ni-filtered Cu $K\alpha$; cell parameters from 48 θ measurements in the range 19–37 $^\circ$; reflections measured for four octants to $2\theta = 140^\circ$ for ranges of h , k and l of 0 to 6, -7 to 7 and -29 to 29, respectively; 3076 reflections mea-

Table 1. Atom coordinates ($\times 10^4$) with e.s.d.'s and equivalent isotropic thermal parameters ($\text{\AA}^2 \times 10^4$)
$$U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	U_{eq}
O1	2148 (4)	2823 (2)	1950 (1)	641
O2	2988 (3)	713 (2)	1293 (1)	501
O3	3681 (3)	1799 (2)	280 (1)	486
O4	3259 (3)	5141 (2)	1340 (1)	600
O5	5617 (3)	5860 (2)	63 (1)	454
O6	7195 (3)	9349 (2)	597 (1)	522
C1	1613 (5)	3773 (3)	1493 (1)	487
C2	1559 (4)	2188 (3)	1082 (1)	457
C3	2643 (4)	3136 (3)	624 (1)	413
C4	4306 (4)	4517 (3)	872 (1)	412
C5	4892 (4)	6361 (3)	568 (1)	402
C6	6709 (5)	7490 (3)	835 (1)	477
C7	2935 (5)	852 (3)	1839 (1)	525
C8	5209 (6)	613 (6)	2044 (1)	844
C9	1325 (6)	-619 (5)	2058 (1)	806

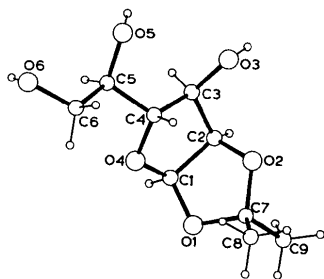


Fig. 1. View of the title compound with atom labels, drawn by the program PLUTO78 (Motherwell & Clegg, 1978).

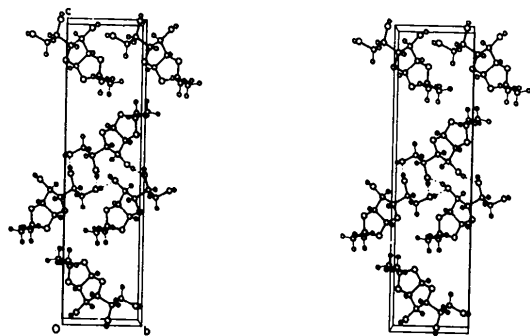


Fig. 2. Stereoscopic view of the crystal structure along a, with b horizontal and c vertical.

sured plus 393 [$F \leq 3\sigma(F)$]; intensity control (86 measurements): average count of 426 with a standard deviation (of the distribution) = 8(1.8%) and no significant trend; no absorption correction; data merged using SHELX76 (Sheldrick, 1976) to give 939 unique reflections with $R_{int} = 0.019$; h, k, l range 0 to 6, 7 and 29; seven reflections with high F_c/F_o ratios, possibly due to extinction, removed; structure solved by direct methods with SHELXS86 (Sheldrick, 1985), non-H atoms refined by least squares (F magnitudes) with anisotropic thermal parameters; 13 H atoms found from difference Fourier syntheses, three in calculated

Table 2. Bond lengths (\AA) and angles ($^\circ$) with e.s.d.'s

C1—O1	1.389 (3)	C4—C5	1.520 (3)
C1—C2	1.515 (3)	C5—O5	1.425 (2)
C1—O4	1.420 (3)	C5—C6	1.511 (3)
C2—O2	1.432 (3)	C6—O6	1.434 (2)
C2—C3	1.505 (3)	C7—O1	1.448 (3)
C3—O3	1.420 (2)	C7—O2	1.422 (2)
C3—C4	1.521 (3)	C7—C8	1.489 (5)
C4—O4	1.435 (2)	C7—C9	1.508 (4)
O1—C1—C2	106.2 (2)	C4—C5—C6	110.4 (2)
O1—C1—O4	112.2 (2)	C4—C5—O5	110.8 (2)
C2—C1—O4	106.3 (2)	O5—C5—C6	108.5 (2)
C1—C2—O2	102.3 (2)	C5—C6—O6	113.4 (2)
C1—C2—C3	104.2 (2)	C1—O1—C7	109.5 (2)
O2—C2—C3	109.5 (2)	C2—O2—C7	108.7 (2)
C2—C3—C4	102.6 (2)	O1—C7—O2	105.5 (2)
C2—C3—O3	114.8 (2)	O1—C7—C8	109.6 (2)
O3—C3—C4	111.4 (2)	O1—C7—C9	108.6 (2)
C3—C4—C5	116.2 (2)	O2—C7—C8	109.2 (2)
C3—C4—O4	104.2 (2)	O2—C7—C9	110.3 (2)
O4—C4—C5	107.5 (2)	C8—C7—C9	113.2 (3)
C1—O4—C4	110.9 (2)		

positions, refined with isotropic thermal parameters; $R = 0.028$, $wR = 0.026$; for final cycle maximum shift/e.s.d. = 0.374 (H) and 0.115, average = 0.021 (all); $w = [\sigma^2(F) + 0.0001F^2]^{-1}$; 200 parameters; difference Fourier synthesis showed a maximum value of 0.09 and a minimum value of $-0.12 e \text{\AA}^{-3}$; atom scattering factors from *International Tables for X-ray Crystallography* (1974).

Fig. 1 shows the molecule and numbering scheme and Fig. 2 a stereoscopic view of the unit-cell contents. Table 1* lists atom parameters; Table 2 gives bond distances and angles. The obtuse angle between the fused rings is $109.8(6)^\circ$, calculated as the angle between the best planes formed by C1, C2 and the atoms bonded directly to them.

Related literature. 1,2:5,6-Di-*O*-isopropylidene- α -D-gulofuranose (Sheldrick, Mackie & Akrigg, 1988).

* Lists of structure amplitudes, thermal parameters, torsion angles, H-atom parameters and least-squares-planes details have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51018 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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