Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* ($Å^2$) *for* (II)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
N1	0.7275 (2)	0.47172 (15)	0.99964 (14)	0.0346 (3)
C2	0.6639 (2)	0.3258 (2)	0.9417 (2)	0.0359 (3)
N2	0.6334 (2)	0.2839 (2)	0.7863 (2)	0.0505 (4)
C3	0.6323 (2)	0.2167 (2)	1.0382 (2)	0.0375 (3)
C4	0.6584 (2)	0.2645 (2)	1.1937 (2)	0.0319 (3)
C41	0.6328 (2)	0.1418 (2)	1.2946 (2)	0.0334 (3)
O41	0.4930 (2)	0.07147 (14)	1.27038 (13)	0.0458 (3)
O42	0.78704 (15)	0.11255 (13)	1.40408 (13)	0.0415 (3)
C42	0.7789 (3)	0.0030 (2)	1.5151 (2)	0.0473 (4)
C5	0.7168 (2)	0.4191 (2)	1.2568 (2)	0.0305 (3)
C51	0.7241 (2)	0.4630 (2)	1.4214 (2)	0.0314 (3)
O51	0.6490 (2)	0.38546 (13)	1.48672 (13)	0.0433 (3)
O52	0.8200 (2)	0.59449 (13)	1.49093 (12)	0.0425 (3)
C52	0.8275 (2)	0.6399 (2)	1.6519 (2)	0.0432 (4)
C6	0.7545 (2)	0.5173 (2)	1.1528 (2)	0.0316 (3)
S61	0.84473 (6)	0.70968 (5)	1.21952 (5)	0.04283 (14)
C61	0.8692 (3)	0.7755 (2)	1.0434 (2)	0.0511 (4)

Table 4. *Selected geometric parameters* (Å, °) *for* (II)

N1—C2	1.340 (2)	O42—C42	1.443 (2)
N1—C6	1.340 (2)	C5—C6	1.413 (2)
N2—C2	1.347 (2)	C5—C51	1.479 (2)
C2—C3	1.406 (2)	O51—C51	1.206 (2)
C3—C4	1.365 (2)	O52—C51	1.332 (2)
C4—C5	1.409 (2)	O52—C52	1.450 (2)
C4—C41	1.502 (2)	S61—C6	1.766 (2)
O41—C41	1.205 (2)	S61—C61	1.796 (2)
O42—C41	1.325 (2)		
C6—C5—C51	127.07 (13)	N1—C6—C5	123.11 (13)
C3—C4—C41—O41	−64.2 (2)	C5—C4—C41—O42	−65.8 (2)
C5—C4—C41—O41	119.7 (2)	N1—C6—S61—C61	−0.40 (14)
C3—C4—C41—O42	110.4 (2)	C5—C6—S61—C61	178.67 (13)

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O51^{i}	0.86	2.20	2.939 (2)	145
N2—H2B···O41^{ii}	0.86	2.33	3.153 (2)	160

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

For both compounds, only a unique data set was collected. The diagrams [Figs. 1(*a*) and (*b*)] were prepared using *ORTEP*II (Johnson, 1976) as implemented in *PLATON* (Spek, 1995*a*) and the packing plots [Figs. 2(*a*) and (*b*), in deposit material] were prepared with *PLUTON* (Spek, 1995*b*). Examination of the structure with *PLATON* showed that there were no solvent-accessible voids in the crystal lattice.

For both compounds, data collection: *CAD-4/PC Software* (Enraf–Nonius, 1992); cell refinement: Enraf–Nonius *SET*4 (de Boer & Duisenberg, 1984) and *CELDIM*; data reduction: *DATRD*2 in *NRCVAX*94 (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to solve structures: *SHELXS*86 (Sheldrick, 1985) for (I); *SOLVER* in *NRCVAX* for (II). For both compounds, program(s) used to refine structures: *NRCVAX*94 and *SHELXL*93 (Sheldrick, 1993); molecular graphics: *NRCVAX*94, *PLATON* and *PLUTON*; software used to prepare material for publication: *NRCVAX*94, *SHELXL*93 and WordPerfect.

GF thanks NSERC (Canada) for Research Grants.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles, together with packing diagrams for both compounds, have been deposited with the IUCr (Reference: AB1308). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1996). C52, 145–148

6-Methoxy-4,5-di(methoxycarbonyl)-2-(2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl)aminopyridine and 4,5-Di(methoxycarbonyl)-6-methylthio-2-(2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl)aminopyridine

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(*Received 16 August 1995; accepted 11 September 1995*)

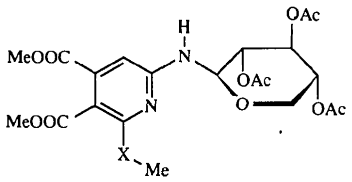
Abstract

The title compounds, dimethyl 2-methoxy-6-(2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl)amino-3,4-pyridinedi-

carboxylate, $C_{21}H_{26}N_2O_{12}$, (III), and dimethyl 2-methylthio-6-(2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl)amino-3,4-pyridinedicarboxylate, $C_{21}H_{26}N_2O_{11}S$, (IV), are isomorphous. Molecules are linked by N—H···O hydrogen bonds [N···O 2.891 (4) Å for (III) and 2.913 (5) Å for (IV)], which generate chains in the *a* direction.

Comment

In a previous paper we reported on the structures and conformation of two related pyridine derivatives, 2-amino-6-methoxy-4,5-di(methoxycarbonyl)pyridine, (I), and 2-amino-4,5-di(methoxycarbonyl)-6-methylthiopyridine, (II) (Low, Ferguson, Cobo, Melguizo, Nogueras & Sánchez, 1996). We report here on the their β-D-xylopyranosyl derivatives, 6-methoxy-4,5-di(methoxycarbonyl)-2-(2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl)aminopyridine, (III), and 4,5-di(methoxycarbonyl)-6-methylthio-2-(2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl)aminopyridine, (IV).



(III) X = O
(IV) X = S

Unlike the parent compounds, (III) and (IV) are isomorphous, which ensures that they have similar packing and conformation. A view of the molecule of (IV) with the atomic numbering scheme is shown in Fig. 1; the corresponding view of compound (III) has been deposited. As anticipated, replacement of one of the amino H atoms in each compound by the β-D-xylopyranosyl moiety (with the consequent removal of a hydrogen-bond donor atom) has had a marked effect on both the conformation of the substituents of the pyridine ring and the crystal packing.

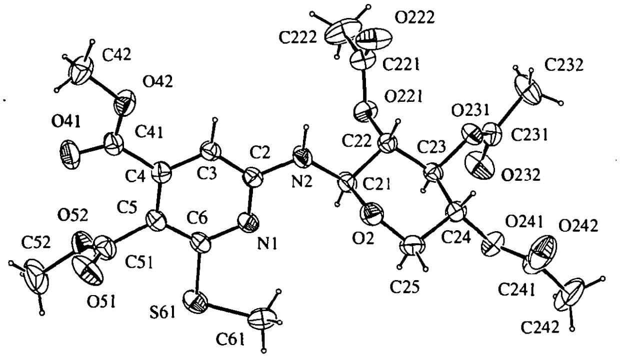


Fig. 1. The molecular structure of (IV) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

There is only one unique hydrogen bond in each structure; molecules are linked by N—H···O hydrogen bonds (Tables 2 and 4) to form chains by translation along the *a* direction. There are no hydrogen bonds linking molecules related by the 2_1 axes.

In the parent compounds (I) and (II), the conformation of the methoxycarbonyl residues at atoms C4 and C5 are quite different [torsion angles C4—C5—C51—O51 of 12.4 (2) in (I) and −16.1 (2)° in (II), and C5—C4—C41—O41 of 81.4 (2) in (I) and 119.7 (2)° in (II)]. The corresponding angles in the title compounds are −76.6 (6) and −10.1 (5)° in (III), and −76.9 (6) and −11.7 (7)° in (IV).

The conformation of the xylopyranoside ring is the usual $^4C_1$ chair form; the β configuration at the anomeric centre was known from the synthesis (Cobo, Melguizo, Sánchez & Nogueras, 1993). The 6-methoxy and 6-methylthio groups are close to being coplanar with the pyridine ring (see the torsion angles in Tables 2 and 4) and in the β-D-xylopyranosyl ring, the conformation of the acetyl side groups is as is usually found, with the carbonyl groups of the acetoxy substituents *cis* to the C—H group of an adjacent ring.

Experimental

Compounds (III) and (IV) were synthesized according to Cobo, Melguizo, Sánchez & Nogueras (1993).

Compound (III)

Crystal data

$C_{21}H_{26}N_2O_{12}$
$M_r = 498.44$
Monoclinic
$P2_1$
$a = 7.8019\ (10)$ Å
$b = 15.889\ (2)$ Å
$c = 10.202\ (2)$ Å
$\beta = 96.24\ (2)°$
$V = 1257.2\ (3)$ Å^3
$Z = 2$
$D_x = 1.317$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 25 reflections
$\theta = 9.5$–$16.5°$
$\mu = 0.109$ mm^{-1}
$T = 294\ (1)$ K
Prism
0.40 × 0.39 × 0.25 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
3015 measured reflections
2827 independent reflections
1818 observed reflections [$I > 2\sigma(I)$]

$R_{\rm int} = 0.014$
$\theta_{\rm max} = 26.9°$
$h = -9 \rightarrow 9$
$k = 0 \rightarrow 20$
$l = 0 \rightarrow 13$
3 standard reflections
frequency: 120 min
intensity decay: no decay, variation 0.8%

Refinement

Refinement on F^2
$R(F) = 0.0417$
$wR(F^2) = 0.1028$

Extinction correction: *SHELXL*93 (Sheldrick, 1993)

$S = 1.009$
2827 reflections
317 parameters
H atoms riding [*SHELXL*93 (Sheldrick, 1993) defaults, C—H 0.96–0.98, N—H 0.86 Å]
$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.156$ e Å^{-3}
$\Delta\rho_{\min} = -0.127$ e Å^{-3}
Extinction coefficient: 0.0093 (21)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
Absolute configuration: Flack (1983) parameter = 0.10 (13)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for* (III)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
N1	0.3222 (3)	0.8857 (2)	0.2812 (3)	0.0505 (7)
C2	0.2300 (4)	0.9548 (2)	0.2987 (3)	0.0454 (7)
N2	0.3123 (3)	1.0205 (2)	0.3692 (3)	0.0592 (8)
C3	0.0594 (4)	0.9652 (2)	0.2445 (3)	0.0448 (7)
C4	−0.0156 (4)	0.9012 (3)	0.1674 (3)	0.0471 (8)
C41	−0.1934 (4)	0.9106 (3)	0.0969 (3)	0.0529 (9)
O41	−0.2527 (4)	0.8644 (3)	0.0131 (3)	0.0925 (10)
O42	−0.2759 (3)	0.9765 (2)	0.1383 (2)	0.0641 (7)
C42	−0.4404 (5)	0.9957 (4)	0.0617 (4)	0.0770 (12)
C5	0.0759 (5)	0.8280 (3)	0.1483 (3)	0.0509 (8)
C51	−0.0007 (5)	0.7524 (3)	0.0785 (4)	0.0644 (10)
O51	−0.0919 (4)	0.7031 (2)	0.1252 (4)	0.0958 (10)
O52	0.0498 (4)	0.7469 (3)	−0.0413 (3)	0.0863 (9)
C52	−0.0169 (8)	0.6739 (4)	−0.1177 (5)	0.126 (2)
C6	0.2459 (4)	0.8253 (3)	0.2079 (3)	0.0510 (8)
O61	0.3346 (3)	0.75373 (15)	0.1904 (3)	0.0655 (7)
C61	0.5084 (5)	0.7488 (3)	0.2505 (5)	0.0742 (11)
C21	0.4836 (4)	1.0129 (3)	0.4318 (3)	0.0501 (8)
O2	0.4815 (3)	0.9788 (2)	0.5608 (3)	0.0619 (7)
C22	0.5691 (4)	1.0991 (2)	0.4483 (3)	0.0452 (7)
O221	0.5802 (3)	1.1373 (2)	0.3219 (2)	0.0572 (6)
C221	0.5036 (5)	1.2123 (3)	0.2975 (4)	0.0665 (10)
O222	0.4208 (5)	1.2460 (3)	0.3739 (4)	0.1070 (12)
C222	0.5362 (7)	1.2447 (4)	0.1662 (5)	0.114 (2)
C23	0.7516 (4)	1.0892 (2)	0.5124 (3)	0.0421 (7)
O231	0.8227 (3)	1.1717 (2)	0.5379 (2)	0.0497 (5)
C231	0.9757 (5)	1.1889 (3)	0.4956 (4)	0.0542 (9)
O232	1.0568 (3)	1.1384 (2)	0.4422 (3)	0.0800 (9)
C232	1.0282 (7)	1.2777 (3)	0.5231 (5)	0.093 (2)
C24	0.7558 (4)	1.0401 (3)	0.6392 (3)	0.0506 (8)
C241	0.9836 (6)	1.0116 (3)	0.8072 (5)	0.0762 (12)
O241	0.9342 (3)	1.0194 (2)	0.6777 (2)	0.0644 (7)
O242	0.8886 (5)	1.0206 (3)	0.8885 (3)	0.1092 (13)
C242	1.1711 (6)	0.9910 (4)	0.8312 (5)	0.119 (2)
C25	0.6518 (5)	0.9601 (3)	0.6187 (4)	0.0649 (10)

Table 2. *Selected geometric parameters (Å, °) for* (III)

N1—C2	1.336 (4)	C4—C5	1.389 (5)
N1—C6	1.318 (4)	C4—C41	1.499 (5)
N2—C2	1.385 (4)	C5—C6	1.398 (5)
C2—C3	1.394 (4)	C5—C51	1.489 (5)
N2—C21	1.422 (4)	O61—C6	1.352 (4)
C3—C4	1.376 (4)	O61—C61	1.428 (5)
C2—N1—C6	117.3 (3)	C5—C4—C41	118.6 (3)
N1—C2—N2	117.6 (3)	C4—C5—C6	116.3 (3)
N1—C2—C3	123.3 (3)	C4—C5—C51	123.8 (3)
N2—C2—C3	119.0 (3)	C6—C5—C51	119.7 (3)
C2—N2—C21	121.9 (3)	N1—C6—O61	118.7 (3)
C2—C3—C4	117.9 (3)	N1—C6—C5	124.9 (3)
C3—C4—C5	120.3 (3)	O61—C6—C5	116.4 (3)
C3—C4—C41	121.0 (3)	C6—O61—C61	117.7 (3)
C5—C4—C41—O41	−10.1 (5)	C22—O221—C221—O222	−3.6 (6)
C4—C5—C51—O51	−76.6 (6)	C23—O231—C231—O232	−2.5 (5)
N1—C6—O61—C61	−1.5 (5)	C24—O241—C241—O242	0.2 (6)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O232$^{\mathrm{i}}$	0.86	2.10	2.891 (4)	151

Symmetry code: (i) $x - 1, y, z$.

Compound (IV)

Crystal data

$C_{21}H_{26}N_2O_{11}S$
$M_r = 514.50$
Monoclinic
$P2_1$
$a = 7.8583$ (9) Å
$b = 15.842$ (2) Å
$c = 10.368$ (2) Å
$\beta = 94.047$ (14)°
$V = 1287.6$ (3) Å^3
$Z = 2$
$D_x = 1.327$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 25 reflections
$\theta = 9.5$–17.5°
$\mu = 0.184$ mm^{-1}
$T = 294$ (1) K
Prism
0.41 × 0.39 × 0.22 mm
Light yellow

Data collection

Enraf–Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
3057 measured reflections
2864 independent reflections
1860 observed reflections [$I > 2\sigma(I)$]
$R_{\mathrm{int}} = 0.009$
$\theta_{\max} = 27.0°$
$h = -10 \rightarrow 9$
$k = 0 \rightarrow 20$
$l = 0 \rightarrow 13$
3 standard reflections frequency: 120 min intensity decay: no decay, variation 1.2%

Refinement

Refinement on F^2
$R(F) = 0.0459$
$wR(F^2) = 0.1131$
$S = 0.993$
2864 reflections
316 parameters
H atoms riding [*SHELXL*93 (Sheldrick, 1993) defaults, C—H 0.96–0.98, N—H 0.86 Å]
$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.166$ e Å^{-3}
$\Delta\rho_{\min} = -0.167$ e Å^{-3}
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
Absolute configuration: Flack (1983) parameter = −0.02 (13)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for* (IV)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
N1	0.3146 (4)	0.9006 (2)	0.2760 (3)	0.0494 (8)
C2	0.2202 (5)	0.9673 (2)	0.2993 (4)	0.0479 (10)
N2	0.3000 (4)	1.0294 (2)	0.3778 (4)	0.0596 (9)
C3	0.0507 (5)	0.9771 (3)	0.2448 (4)	0.0467 (9)
C4	−0.0200 (5)	0.9148 (3)	0.1628 (4)	0.0482 (9)
C41	−0.1978 (6)	0.9244 (3)	0.0919 (4)	0.0545 (10)
O41	−0.2543 (4)	0.8815 (3)	0.0030 (4)	0.0902 (12)
O42	−0.2826 (4)	0.9882 (2)	0.1370 (3)	0.0656 (8)
C42	−0.4467 (6)	1.0077 (4)	0.0630 (5)	0.082 (2)
C5	0.0755 (5)	0.8430 (3)	0.1402 (4)	0.0503 (10)
C51	−0.0051 (6)	0.7690 (3)	0.0644 (5)	0.0661 (13)
O51	−0.0974 (5)	0.7197 (2)	0.1064 (5)	0.0979 (13)

O52	0.0520 (5)	0.7630 (3)	−0.0497 (3)	0.0879 (11)
C52	−0.0103 (9)	0.6881 (5)	−0.1238 (6)	0.119 (3)
C6	0.2435 (5)	0.8402 (3)	0.1972 (4)	0.0489 (9)
S61	0.3733 (2)	0.75373 (8)	0.16581 (11)	0.0662 (3)
C61	0.5625 (6)	0.7720 (3)	0.2744 (5)	0.0695 (13)
C21	0.4714 (5)	1.0224 (3)	0.4379 (4)	0.0519 (10)
O2	0.4722 (4)	0.9864 (2)	0.5643 (3)	0.0621 (8)
C22	0.5573 (5)	1.1088 (3)	0.4555 (4)	0.0458 (9)
O221	0.5657 (4)	1.1471 (2)	0.3311 (2)	0.0582 (8)
C221	0.4875 (6)	1.2222 (3)	0.3073 (4)	0.0623 (12)
O222	0.4027 (5)	1.2543 (3)	0.3797 (4)	0.0957 (12)
C222	0.5212 (7)	1.2561 (5)	0.1780 (5)	0.108 (2)
C23	0.7391 (5)	1.0976 (2)	0.5173 (4)	0.0445 (9)
O231	0.8100 (3)	1.1806 (2)	0.5420 (2)	0.0491 (6)
C231	0.9579 (6)	1.1991 (3)	0.4978 (4)	0.0539 (11)
O232	1.0377 (4)	1.1490 (2)	0.4426 (4)	0.0819 (10)
C232	1.0066 (8)	1.2895 (4)	0.5223 (6)	0.085 (2)
C24	0.7457 (5)	1.0491 (3)	0.6435 (4)	0.0519 (10)
O241	0.9238 (4)	1.0278 (2)	0.6810 (3)	0.0680 (9)
C241	0.9775 (6)	1.0251 (4)	0.8085 (6)	0.0753 (15)
O242	0.8848 (5)	1.0384 (4)	0.8884 (4)	0.1063 (14)
C242	1.1610 (7)	1.0024 (5)	0.8330 (7)	0.122 (3)
C25	0.6431 (6)	0.9677 (3)	0.6206 (5)	0.0659 (13)

Table 4. *Selected geometric parameters (Å, °) for* (IV)

N1—C2	1.323 (5)	C4—C5	1.391 (6)
N1—C6	1.353 (5)	C4—C41	1.540 (6)
N2—C2	1.396 (5)	C5—C6	1.408 (6)
C2—C3	1.418 (6)	C5—C51	1.525 (6)
N2—C21	1.448 (5)	S61—C6	1.752 (4)
C3—C4	1.393 (6)	S61—C61	1.823 (5)
C2—N1—C6	117.6 (3)	C3—C4—C41	122.1 (4)
N1—C2—N2	115.8 (3)	C4—C5—C6	117.2 (3)
N1—C2—C3	122.5 (3)	C4—C5—C51	120.4 (4)
N2—C2—C3	121.7 (3)	C6—C5—C51	122.3 (4)
C2—N2—C21	124.3 (3)	N1—C6—C5	124.4 (4)
C2—C3—C4	119.3 (4)	N1—C6—S61	116.4 (3)
C3—C4—C5	119.0 (4)	S61—C6—C5	119.2 (3)
C5—C4—C41	118.9 (4)	C6—S61—C61	102.8 (2)
C5—C4—C41—O41	−11.7 (7)	C22—O221—C221—O222	−6.0 (7)
C4—C5—C51—O51	−76.9 (6)	C23—O231—C231—O232	−2.9 (6)
N1—C6—S61—C61	7.1 (4)	C24—O241—C241—O242	0.9 (8)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O232^{i}	0.86	2.11	2.913 (5)	157

Symmetry code: (i) $x - 1, y, z$.

It was not possible to determine the absolute configuration of molecules (III) and (IV) from the X-ray data, but the absolute configuration of the β-D-xylopyranosyl moiety was known from the synthetic work and the coordinates were chosen to have this known configuration. The diagram of (IV) (Fig. 1) was prepared using *ORTEP*II (Johnson, 1976) as implemented in *PLATON* (Spek, 1995*a*). The packing diagram (deposited figure) of (III) was prepared using *PLUTON* (Spek, 1995*b*). Examination of the structures with *PLATON* showed that there were no solvent-accessible voids in the crystal lattices.

For both compounds, data collection: *CAD*-4/*PC Software* (Enraf–Nonius, 1992); cell refinement: Enraf–Nonius *SET*4 (de Boer & Duisenberg, 1984) and *CELDIM*; data reduction: *DATRD*2 in *NRCVAX*94 (Gabe, Le Page, Charland, Lee & White, 1989); program(s) used to solve structures: *SOLVER* in *NRCVAX*; program(s) used to refine structures: *NRCVAX*94 and *SHELXL*93 (Sheldrick, 1993); molecular graphics: *NRCVAX*94, *PLATON* and *PLUTON*; software used to prepare material for publication: *NRCVAX*94, *SHELXL*93 and WordPerfect.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles, together with a displacement ellipsoid plot (30% probability) and a packing diagram for compound (III), have been deposited with the IUCr (Reference: AB1310). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2-Methylthio-5-nitroso-6-*N*-(2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl)amino-4(3*H*)-pyrimidinone

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Abstract

The title compound, $C_{16}H_{20}N_4O_9S$, has a strong intramolecular N—H···O hydrogen bond between the nitrosyl O atom and an adjacent N—H moiety [N···O 2.516 (8) Å]. The β-D-xylopyranosyl ring has a $^4C_1$ conformation, with all non-H substituents in equatorial positions. Molecules are linked about 2_1 axes *via* intermolecular N—H···O hydrogen bonds [N···O 2.892 (8) Å].