Crystal structure of (2′*R**,3′*R**,4′*R**,5′*R**,6′*R**)-1-(6′-hydroxy-5′-methoxy-2′,3′,4′,5′-tetrahydro-2′,4′-heptanofuran-3′-yl)-5-methyl-(1*H*,3*H*)-pyrimidine-2,4-dione, $[C_4H_4O(OCH_3)(C_5H_5N_2O_2)](C_7H_{13}OH)$

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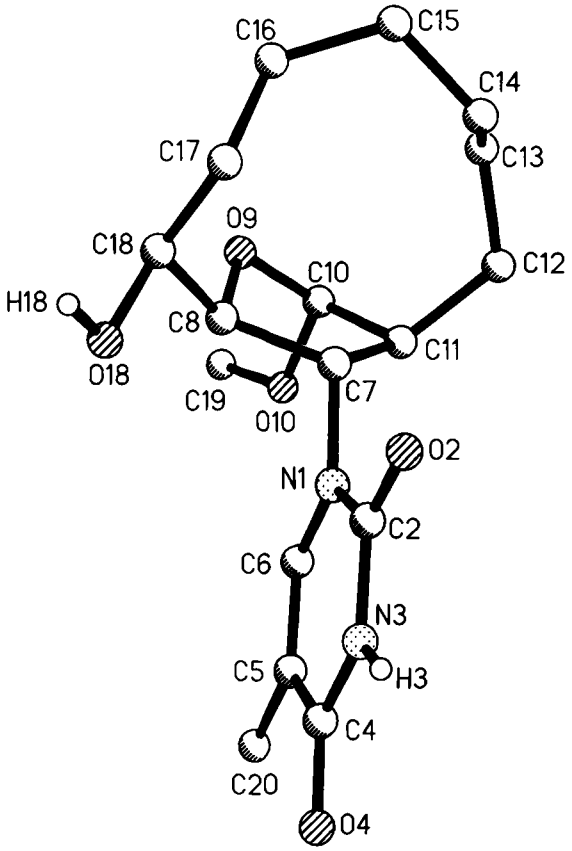

Abstract

$C_{17}H_{26}N_2O_5$, monoclinic, $P12_1/n1$ (No. 14), $a = 10.481(1)$ Å, $b = 17.158(1)$ Å, $c = 10.525(1)$ Å, $\beta = 106.11(1)°$, $V = 1818.4$ Å^3, $Z = 4$, $R_{gt}(F) = 0.055$, $wR_{ref}(F^2) = 0.157$, $T = 293$ K.

Source of material

The title compound was prepared as described in ref. 1

Discussion

The intermolecular hydrogen bridges O4···H3 (194 pm) around a symmetry centre form a dimer of the molecule. These dimers are connected by the hydrogen bridges O2···H18 forming an infinite zigzag chain parallel [100].

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.5 × 0.5 × 0.6 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.91 cm^{-1}
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4370, 4154
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3259
$N(param)_{refined}$:	225
Programs:	SHELXS-97 [2], SHELXL-97 [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(3)	4*e*	0.388(3)	0.542(1)	0.495(3)	0.08
H(6)	4*e*	0.1414	0.5988	0.0886	0.08
H(7)	4*e*	0.0108	0.6588	0.3487	0.08
H(8)	4*e*	–0.0639	0.5586	0.1320	0.08
H(10)	4*e*	–0.1540	0.7521	0.0256	0.08
H(11)	4*e*	0.0917	0.7294	0.1542	0.08
H(12A)	4*e*	0.0665	0.8028	0.3317	0.08
H(12B)	4*e*	–0.0077	0.8414	0.1972	0.08
H(13A)	4*e*	–0.2056	0.7802	0.2358	0.08
H(13B)	4*e*	–0.1542	0.8598	0.3026	0.08
H(14A)	4*e*	–0.0549	0.7318	0.4591	0.08
H(14B)	4*e*	–0.1036	0.8111	0.5027	0.08
H(15A)	4*e*	–0.3228	0.7701	0.4225	0.08
H(15B)	4*e*	–0.2416	0.7154	0.5350	0.08
H(16A)	4*e*	–0.3023	0.6779	0.2636	0.08
H(16B)	4*e*	–0.3800	0.6443	0.3586	0.08
H(17A)	4*e*	–0.1132	0.6110	0.4423	0.08
H(17B)	4*e*	–0.2322	0.5549	0.4364	0.08
H(18A)	4*e*	–0.2572	0.5347	0.2093	0.08
H(18)	4*e*	–0.122(3)	0.460(2)	0.359(3)	0.08
H(19A)	4*e*	–0.0861	0.6379	–0.2190	0.08
H(19B)	4*e*	–0.1733	0.7087	–0.1999	0.08
H(19C)	4*e*	–0.2021	0.6253	–0.1539	0.08
H(20A)	4*e*	0.4430	0.5442	0.0768	0.08
H(20B)	4*e*	0.2962	0.5455	–0.0133	0.08

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	4*e*	0.1504(1)	0.60704(8)	0.2798(1)	0.0355(6)	0.0492(7)	0.0355(6)	0.0091(5)	0.0107(5)	0.0058(5)
C(2)	4*e*	0.2237(1)	0.58980(9)	0.4071(1)	0.0380(7)	0.0405(8)	0.0354(7)	0.0020(6)	0.0105(6)	0.0031(6)
O(2)	4*e*	0.1904(1)	0.60780(7)	0.5052(1)	0.0497(6)	0.0609(7)	0.0361(6)	0.0106(5)	0.0143(5)	0.0008(5)
N(3)	4*e*	0.3407(1)	0.55121(8)	0.4158(1)	0.0387(7)	0.0528(8)	0.0348(6)	0.0088(6)	0.0074(5)	0.0036(5)
C(4)	4*e*	0.3888(2)	0.52709(9)	0.3131(2)	0.0388(7)	0.0417(8)	0.0406(8)	0.0043(6)	0.0112(6)	0.0011(6)
O(4)	4*e*	0.4943(1)	0.49145(8)	0.3351(1)	0.0477(6)	0.0691(8)	0.0472(6)	0.0220(6)	0.0119(5)	0.0028(6)
C(5)	4*e*	0.3079(2)	0.54772(9)	0.1821(2)	0.0433(8)	0.0472(9)	0.0378(7)	0.0053(6)	0.0134(6)	0.0017(6)
C(6)	4*e*	0.1941(2)	0.5858(1)	0.1726(2)	0.0423(8)	0.0520(9)	0.0341(7)	0.0062(7)	0.0112(6)	0.0054(6)
C(7)	4*e*	0.0219(1)	0.64667(9)	0.2614(2)	0.0344(7)	0.0453(8)	0.0407(7)	0.0074(6)	0.0126(6)	0.0053(6)
C(8)	4*e*	-0.0963(2)	0.5962(1)	0.1858(2)	0.0390(7)	0.0539(9)	0.0417(8)	0.0016(7)	0.0132(6)	0.0044(7)
O(9)	4*e*	-0.1836(1)	0.64957(8)	0.0982(1)	0.0363(6)	0.0785(9)	0.0492(7)	0.0035(5)	0.0088(5)	0.0157(6)
C(10)	4*e*	-0.1031(2)	0.7049(1)	0.0588(2)	0.0435(8)	0.069(1)	0.055(1)	0.0122(8)	0.0148(7)	0.0233(8)
O(10)	4*e*	-0.0452(1)	0.6747(1)	-0.0363(1)	0.0505(7)	0.104(1)	0.0458(7)	0.0091(7)	0.0151(5)	0.0201(7)
C(11)	4*e*	0.0103(2)	0.7232(1)	0.1817(2)	0.0433(8)	0.0492(9)	0.058(1)	0.0057(7)	0.0161(7)	0.0139(8)
C(12)	4*e*	-0.0096(2)	0.7975(1)	0.2548(3)	0.080(2)	0.048(1)	0.092(2)	0.010(1)	0.025(1)	0.009(1)
C(13)	4*e*	-0.1328(3)	0.8049(1)	0.3008(3)	0.091(2)	0.058(1)	0.092(2)	0.025(1)	0.031(1)	0.005(1)
C(14)	4*e*	-0.1259(3)	0.7700(2)	0.4370(2)	0.104(2)	0.071(1)	0.076(2)	0.026(1)	0.032(1)	-0.010(1)
C(15)	4*e*	-0.2520(3)	0.7319(2)	0.4445(3)	0.099(2)	0.099(2)	0.084(2)	0.039(2)	0.048(2)	0.004(1)
C(16)	4*e*	-0.2934(2)	0.6616(2)	0.3539(3)	0.062(1)	0.099(2)	0.083(2)	0.014(1)	0.037(1)	0.007(1)
C(17)	4*e*	-0.1974(2)	0.5926(1)	0.3859(2)	0.063(1)	0.070(1)	0.060(1)	0.0000(9)	0.0345(9)	0.0092(9)
C(18)	4*e*	-0.1716(2)	0.5512(1)	0.2682(2)	0.055(1)	0.057(1)	0.057(1)	-0.0061(8)	0.0258(8)	0.0026(8)
O(18)	4*e*	-0.0916(2)	0.48393(9)	0.3073(2)	0.107(1)	0.0604(9)	0.094(1)	0.0128(9)	0.062(1)	0.0213(8)
C(19)	4*e*	-0.1338(3)	0.6605(2)	-0.1624(2)	0.073(2)	0.172(3)	0.051(1)	0.009(2)	0.012(1)	0.014(2)
C(20)	4*e*	0.3549(2)	0.5244(1)	0.0660(2)	0.063(1)	0.071(1)	0.0449(9)	0.0164(9)	0.0236(8)	0.0019(8)

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