# Crystal structure of (3a*R*,5*S*,6*R*,6a*R*)-6-hydroxy-5-hydroxymethyl-perhydrofuro[3,2-*b*]furan-2-one, $C_7H_{10}O_5$

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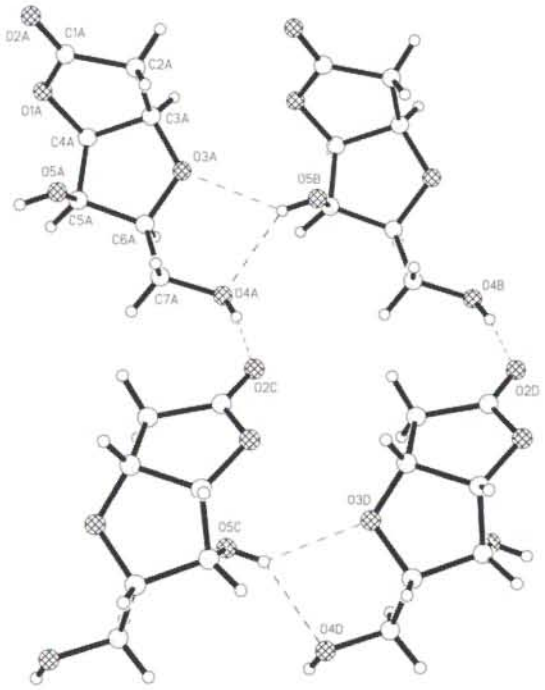


## Abstract

$C_7H_{10}O_5$, monoclinic, $P12_11$ (No. 4), $a = 5.197(1)$ Å, $b = 14.526(3)$ Å, $c = 5.659(1)$ Å, $\beta = 117.08(1)°$, $V = 380.4$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.038$, $R_w(F^2) = 0.078$, $T = 293$ K.

## Source of material

The title compound (alternative name (+)-3,6-anhydro-2-deoxy-L-*galacto*-1,4-heptonolactone [1]) was prepared by Pd(II)-catalyzed oxycarbonylation of (2*S*,3*S*,4*S*)-5-hexene-1,2,3,4-tetrol in acetic acid [1-3]. The lactone was recrystallized from ethyl acetate to form colorless crystals, (mp 398 K – 399 K, $[\alpha]_D^{24} = 90.6$, $c = 1.15$, $CH_3OH$).

## Discussion

In the crystal, there is parallel stacking of the molecules. This could be a result of the complex network of intermolecular hydrogen bonds wich are evident in the crystal structure. A four molecule-interaction could be defined. The O(5)–H(5)···O(4) and O(5)–H(5)···O(3) distances are 2.240 Å and 2.326 Å. The O(4)–H(4)···O(2) distance is 1.967 Å.

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | colorless block, size 0.15 x 0.3 x 0.4 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 1.31 cm$^{-1}$ |
| Diffractometer, scan mode: | Nicolet P3, Wyckoff |
| $2\theta_{max}$: | 54.96° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 1026, 900 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 821 |
| $N(param)_{refined}$: | 112 |
| Programs: | SHELXS-86 [4], SHELXL-93 [5] |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(2A) | 2*a* | 1.4451(7) | 0.9960(3) | 1.4937(5) | 0.058 |
| H(2B) | 2*a* | 1.2726(7) | 0.9081(3) | 1.5044(5) | 0.058 |
| H(3) | 2*a* | 0.8996(6) | 0.9921(2) | 1.4673(6) | 0.051 |
| H(4) | 2*a* | 1.355(6) | 1.324(3) | 1.826(5) | 0.1 |
| H(4A) | 2*a* | 0.6472(6) | 1.0560(2) | 1.0589(6) | 0.051 |
| H(5) | 2*a* | 1.227(2) | 1.166(3) | 0.973(3) | 0.072 |
| H(5A) | 2*a* | 0.8302(6) | 1.1899(2) | 0.9695(5) | 0.05 |
| H(6) | 2*a* | 0.8253(6) | 1.2020(2) | 1.3747(6) | 0.052 |
| H(7A) | 2*a* | 1.4052(7) | 1.2492(2) | 1.5279(6) | 0.059 |
| H(7B) | 2*a* | 1.1469(7) | 1.3170(2) | 1.3716(6) | 0.059 |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| O(1) | 2*a* | 0.9301(4) | 0.9917(2) | 0.9643(4) | 0.043(1) | 0.062(1) | 0.032(1) | 0.003(1) | 0.0117(8) | −0.0077(9) |
| C(1) | 2*a* | 1.1736(6) | 0.9460(2) | 1.1216(5) | 0.041(1) | 0.052(2) | 0.038(1) | −0.005(1) | 0.018(1) | −0.001(1) |
| O(2) | 2*a* | 1.2900(5) | 0.8984(2) | 1.0268(4) | 0.061(1) | 0.068(2) | 0.051(1) | 0.012(1) | 0.027(1) | −0.004(1) |
| C(2) | 2*a* | 1.2597(7) | 0.9650(3) | 1.4099(5) | 0.050(2) | 0.059(2) | 0.035(1) | −0.001(2) | 0.017(1) | 0.004(1) |

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**Table 3.** Continued.

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| O(3) | 2*a* | 1.1319(5) | 1.1087(2) | 1.5579(4) | 0.077(2) | 0.046(1) | 0.032(1) | –0.014(1) | 0.024(1) | –0.000(1) |
| C(3) | 2*a* | 1.0238(6) | 1.0258(2) | 1.4089(6) | 0.047(2) | 0.049(2) | 0.037(1) | –0.013(1) | 0.024(1) | –0.004(1) |
| O(4) | 2*a* | 1.2118(6) | 1.2924(2) | 1.7392(5) | 0.080(2) | 0.068(2) | 0.056(1) | –0.021(2) | 0.035(1) | –0.017(1) |
| C(4) | 2*a* | 0.8560(6) | 1.0555(2) | 1.1170(6) | 0.031(1) | 0.059(2) | 0.038(1) | 0.000(1) | 0.015(1) | –0.005(1) |
| O(5) | 2*a* | 1.2419(4) | 1.1472(2) | 1.1152(4) | 0.044(1) | 0.067(1) | 0.038(1) | 0.002(1) | 0.0223(8) | 0.011(1) |
| C(5) | 2*a* | 0.9692(6) | 1.1523(2) | 1.1156(5) | 0.034(1) | 0.055(2) | 0.031(1) | 0.008(1) | 0.012(1) | 0.008(1) |
| C(6) | 2*a* | 1.0135(6) | 1.1865(2) | 1.3847(6) | 0.042(1) | 0.052(2) | 0.039(1) | 0.000(1) | 0.021(1) | 0.001(1) |
| C(7) | 2*a* | 1.2115(7) | 1.2661(2) | 1.4960(6) | 0.056(2) | 0.047(2) | 0.041(2) | –0.004(2) | 0.020(1) | 0.003(1) |

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