

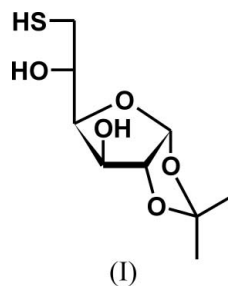
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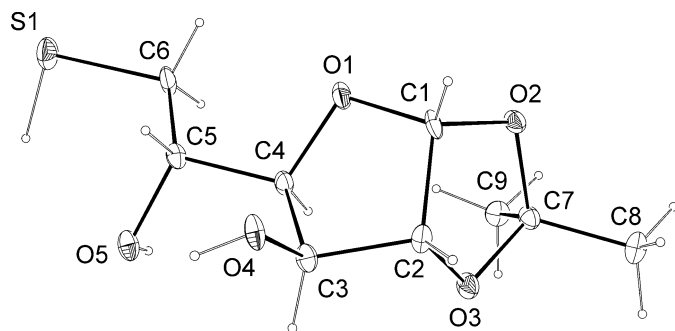
## Key indicators

Single-crystal X-ray study  
 $T = 100$  K  
Mean  $\sigma(C-C) = 0.006$  Å  
 $R$  factor = 0.052  
 $wR$  factor = 0.130  
Data-to-parameter ratio = 15.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.1,2-*O*-Isopropylidene-6-thio- $\alpha$ -D-glucofuranoseIn the crystalline state, the title compound,  $C_9H_{16}O_5S$ , forms  
hydrogen-bonded chains.Received 6 November 2006  
Accepted 20 November 2006

## Comment

The title compound, (I), was prepared as part of a project  
aimed at the synthesis of potential gelators of organic solvents  
(Luboradzki *et al.*, 2005). The class of saccharide-based gela-  
tors having free OH groups and a glucofuranose fragment are  
able to form gels with a huge spectrum of organic solvents.  
According to the driving forces responsible for molecular  
aggregation, they may be classified as hydrogen-bond-based  
gelators (Terech & Weiss, 1997).

The molecular structure of (I) with the atom-labelling scheme is shown in Fig. 1. The molecules are bound into one-dimensional hydrogen-bonded chains (generated by the screw axis along the  $b$  axis) utilizing two hydroxy H atoms [O4—H4O $\cdots$ O5( $-x + 1, y + \frac{1}{2}, -z + 1$ ) and O5—H5O $\cdots$ O4( $x, y - 1, z$ )]. The hydrogen-bond distances are 2.679 (4) and 1.90 (4) Å for O4 $\cdots$ O5 and H4O $\cdots$ O5, and 2.765 (4) Å and 2.08 (5) for O5 $\cdots$ O4 and H5O $\cdots$ O4. The O4—H4O $\cdots$ O5 and O5—H5O $\cdots$ O4 angles are 160 (4) and 161 (5) $^\circ$ , respectively. The S—H H atom is not involved in any hydrogen bonds. There are at least five crystal structures containing the  $\alpha$ -D-glucofuranose fragment reported in the literature [CONQUEST, Version 1.8 (Bruno *et al.*, 2002); Cambridge Structural Database, Version 5.27 (Allen, 2002)] but none having —SH instead of —OH. Molecules in all the previously reported structures form hydrogen-bonded networks in which each molecule takes part in six hydrogen bonds (three as a donor and three as an acceptor), while molecules of (I) are involved in four hydrogen bonds (two as a donor and two as an acceptor). This is probably the cause of the significantly lower melting point of (I) (354–356 K) in comparison with the similar compound 1,2-*O*-isopropylidene- $\alpha$ -D-glucofuranose (432–433 K). The five-membered glucofuranose ring of (I) adopts a  $^3T_4$  conformation.



**Figure 1**

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as circles of arbitrary radii.

## Experimental

The title compound was prepared as described previously (Nifantsev *et al.*, 1978) and recrystallized from acetonitrile at 291 K.

### Crystal data

$C_9H_{16}O_5S$	$Z = 2$
$M_r = 236.28$	$D_x = 1.452 \text{ Mg m}^{-3}$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 9.1655 (8) \text{ \AA}$	$\mu = 0.30 \text{ mm}^{-1}$
$b = 5.8452 (5) \text{ \AA}$	$T = 100 (1) \text{ K}$
$c = 10.5282 (9) \text{ \AA}$	Poor quality needle, colourless
$\beta = 106.563 (4)^\circ$	$0.5 \times 0.1 \times 0.1 \text{ mm}$
$V = 540.58 (8) \text{ \AA}^3$	

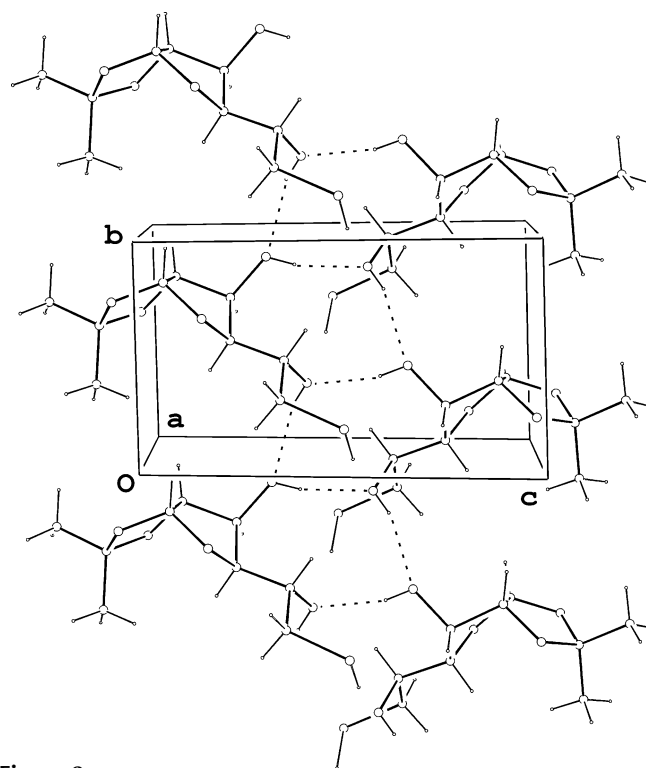
### Data collection

Nonius KappaCCD diffractometer	2324 independent reflections
$\varphi$ scans	2020 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.060$
3891 measured reflections	$\theta_{\text{max}} = 27.6^\circ$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 1.2765P]$
$R[F^2 > 2\sigma(F^2)] = 0.052$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.130$	$(\Delta/\sigma)_{\text{max}} = 0.010$
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.40 \text{ e \AA}^{-3}$
2324 reflections	$\Delta\rho_{\text{min}} = -0.45 \text{ e \AA}^{-3}$
150 parameters	Absolute structure: Flack (1983),
H atoms treated by a mixture of independent and constrained refinement	955 Freidel pairs
	Flack parameter: $-0.04 (15)$

H atoms were geometrically constrained to ride on their parent atom [ $C-H = 0.96-0.98 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ ], except those from  $-SH$  and  $-OH$  groups which were located in difference Fourier syntheses and refined isotropically [ $S1-H1S = 1.41 (6) \text{ \AA}$ ,  $O4-H4O = 0.80 (4) \text{ \AA}$  and  $O5-H5O = 0.71 (5) \text{ \AA}$ ]. The absolute configuration determined from anomalous scattering effects is as expected from the synthesis.



**Figure 2**

The packing of (I), viewed down the  $a$  axis. Hydrogen-bonded contacts are shown as dashed lines.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

## References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.  
 Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* **B58**, 389–397.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
 Luboradzki, R., Pakulski, Z. & Sartowska, B. (2005). *Tetrahedron*, **61**, 10122–10128.  
 Nifantsev, E. E., Koroteev, M. P., Ermouskhina, S. A., Lysenko, K. A. & Kochetkov, N. K. (1978). *Zh. Obshch. Khim.* **48**, 1904.  
 Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.  
 Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.  
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.  
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.  
 Terech, P. & Weiss, R. G. (1997). *Chem. Rev.* **97**, 3133–3159.