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1,3,4,6-Tetra-*O*-acetyl-2-*O*-benzyl-α-D-mannopyranose

Qi An* and Shende Jiang

School of Pharmaceutical Science and Technology, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail: zhangdebin@netease.com

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.007 Å
R factor = 0.043
wR factor = 0.104
Data-to-parameter ratio = 7.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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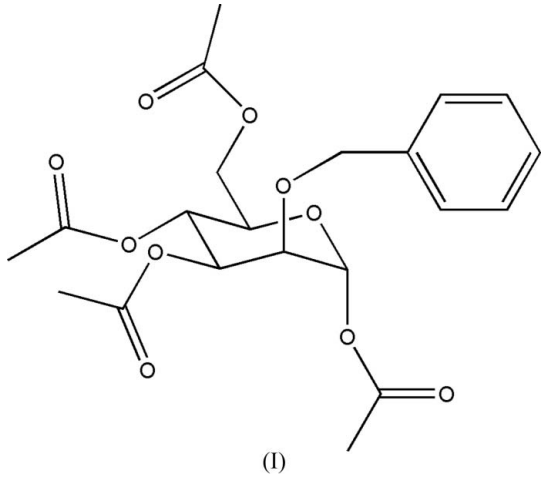
In the title compound, $C_{21}H_{26}O_{10}$, the pyranose ring adopts a chair conformation.

Comment

The title compound, (I) (Ogawa & Sasajima, 1981), is a key intermediate in the synthesis of 2-deoxy-2-[^{18}F]fluoro-D-glucose ([^{18}F]FDG; Hamacher *et al.*, 1986), a compound which measures glucose cellular uptake in the body and is one of the most widely used molecular imaging probes in positron emission tomography (PET). In the crystal structure, the pyranose ring of (I) adopts a chair conformation (Fig. 1).



(I)

Experimental

2-*O*-Benzyl-D-mannopyranose (0.5 g, 1.4 mmol) and 4-dimethylaminopyridine (50 mg, 0.46 mol) were added with stirring to pyridine (30 ml) at room temperature. Acetic anhydride (5.4 ml, 5.5 mmol) was then added dropwise and the reaction mixture was stirred at room temperature for 24 h. The pyridine solvent was removed by vacuum evaporation at 333 K then co-evaporated with toluene. The residue was purified by column chromatography (ethyl acetate/petroleum ether 1:2) to obtain the product (yield 0.58 g, 95%). Single crystals of (I) (m.p. 348–349 K) were obtained by slow evaporation of an ethyl acetate and petroleum ether (1:2) solution.

Crystal data

$C_{21}H_{26}O_{10}$
M_r = 438.42
Monoclinic, $P2_1$
a = 7.855 (6) Å
b = 10.138 (8) Å
c = 13.949 (10) Å
β = 94.612 (14)°
V = 1107.3 (14) Å^3
Z = 2
D_x = 1.315 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 294 (2) K
Block, colourless
0.26 × 0.24 × 0.22 mm

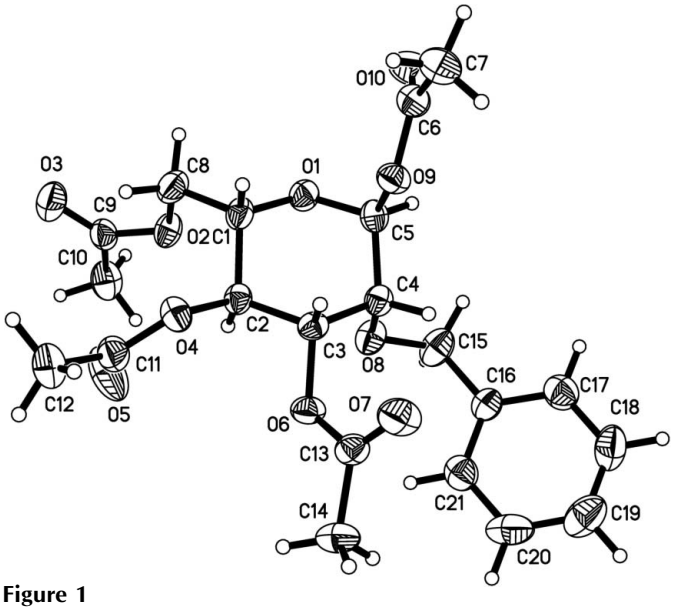


Figure 1
The molecular structure of (I) showing displacement ellipsoids drawn at the 30% probability level for non-H atoms.

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.973, T_{max} = 0.977
5692 measured reflections
2076 independent reflections
1345 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.104
S = 1.01
2076 reflections
284 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93 (aromatic), 0.96 (methyl), 0.97 (CH_2) and 0.98 Å (CH), and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate about their local threefold axes. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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