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X-ray structure of the dipotassium salt of D-mannose 1-phosphate 3.25 hydrate

Lucjan B. Jerzykiewicz,* Tadeusz Lis and Ewa Zuziak

Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, Pl-50-383 Wrocław, Poland

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Abstract—The first crystal structure of mannose 1-phosphate is described. The dipotassium hydrate salt crystallizes in the $P2_12_12$ space group. There are two independent dianions (**I** and **II**) in the asymmetric unit, which are α anomers adopting the $^4C_1$ chair conformation. The main difference between the two mannose 1-phosphate dianions is the orientation of the phosphate group with relation to the pyranosyl ring. In **I**, one of the phosphate oxygen atoms is antiperiplanar positions with respect to carbon atom C-1, whereas the two others are situated synclinally. The corresponding orientations of the terminal phosphate oxygen atoms in **II** are synperiplanar and anticlinal. The potassium cations are six- and seven-coordinate, mainly with O atoms of hydroxyl groups and water molecules. There are potassium channels extending along the *c*-axis. In the packing arrangement, water molecules and mannose phosphate groups also define two different types of layers parallel to *a*-axis. Within water channels there are extensive hydrogen-bonding networks.

Keywords: X-ray crystal structure; D-Mannose 1-phosphate; Sugar phosphates

1. Introduction

The phosphate esters of carbohydrates occur widely in living organisms,[1,2] serving as energy reservoirs, fuels and metabolic intermediates, structural framework constituents for RNA and DNA, and also components of proteins and lipids.[2,3]

This paper describes the first crystal structure of the mannose 1-phosphate (Man-1-P) molecule, which is a conversion product of mannose 6-phosphate caused by the specific enzyme phosphomannomutase in all living cells. Mannose 1-phosphate is essential for glycoprotein biosynthesis and a lack of it causes mental retardation.[4]

2. Results and discussion

The asymmetric unit of the title crystal consists of the two crystallographically independent mannose 1-phosphate dianions (**I** and **II**), four potassium cations and six and a half water molecules (one being positionally disordered between two sets of sites with the occupancy factor of 0.5). The molecular structure and atom-numbering scheme of one dianion are presented in Figure 1. Processing of crystal data and refinement details for the crystal are given in Table 1. Cremer–Pople puckering parameters[5] and the molecular geometry are listed in Tables 2 and 3, respectively.

The hexapyranosyl ring of each anion adopts the $^4C_1$ (D) chair conformation. This arrangement corresponds well with theoretical calculations[6] as well as with experimental data for other sugar phosphates such as: disodium D-glucose 1-phosphate,[7] dipotassium D-glucose 1-phosphate,[8] barium D-glucose 6-phosphate,[9] sodium hydrogen D-glucose 6-phosphate[10] and galactose 1-phosphate pentahydrate.[11] The torsion angles (Table 3) confirm in both anions (**I** and **II**) the α anomeric form of the saccharide moieties. It is noteworthy that α anomers are not as frequently observed as β anomers.[6] As in other known phosphate esters[7,8,12] the conformation about the exocyclic C-5–C-6 bond in both anions is

* Corresponding author. Tel.: +48 71 3757433; fax: +48 71 3204338; e-mail: jerzyk@wchuwr.chem.uni.wroc.pl

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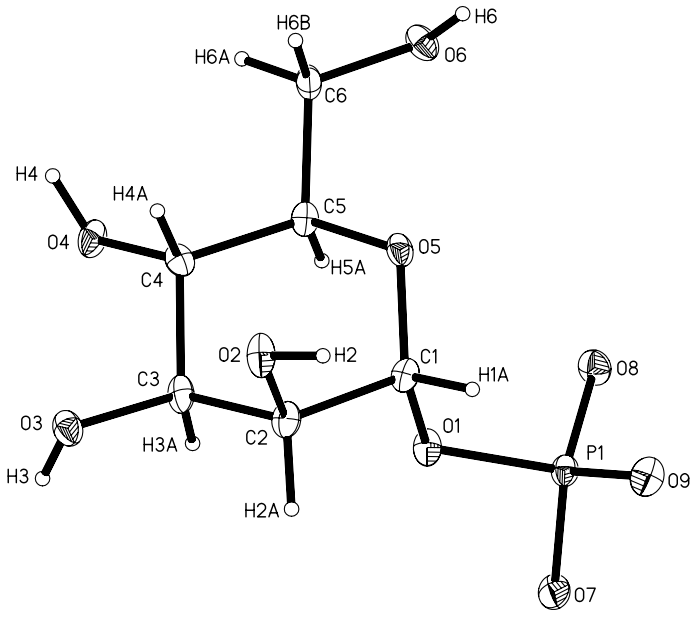

Figure 1. The molecular structure of the mannose 1-phosphate anion (**I**) showing 50% probability displacement ellipsoids and atom-numbering scheme.

Table 1. Crystallographic data

Empirical formula	$4(C_6H_{11}O_9K_2P\ 3.25H_2O)$
Molecular weight	1579.48
Crystal size (mm)	$0.45 \times 0.25 \times 0.02$
Crystal system	Orthorhombic
Space group	$P2_12_12$ (No 18)
Z	2
a (Å)	8.984(3)
b (Å)	43.216(8)
c (Å)	7.410(3)
V (Å^3)	2877(2)
D_c (g cm^{-3})	1.823
$F(000)$	1636
μ (mm^{-1})	0.831
λ (Mo K$_\alpha$) (Å)	0.71073
Temperature (K)	100(2)
$2\theta_{max}$ (°)	33
R_{int} (on F^2)	0.0653
Reflections measured	43,101
Unique reflections	10,096
Number of observed reflections [$I > 2\sigma(I)$]	8658
Final R_1 indices [$I > 2\sigma(I)$][a]	0.0535
Final wR_2[b]	0.0912
Final R_1 indices (all data)	0.0660
Final wR_2 indices (all data)	0.0965
Goodness of fit S	1.061
Largest diff. peak and hole (e Å^{-3})	0.71 and −0.54

[a] $R_1 = \sum(F_o - F_c)/\sum F_o$.
[b] $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]\big/\sum[w(F_o^2)^2]\}^{1/2}$.

antiperiplanar. The endocyclic angles as well as C–O and the C–C bond lengths are characteristic for pyranose rings,[6,13] and the ester bond lengths of **I** and **II** are also typical for diionized phosphate groups in the monophosphate esters.[3,8,11,14] Moreover the hydroxyl groups connected to C-3 and C-4 (C-31 and C-41 in **II**) are in equatorial orientation.

The most interesting feature of the mannose 1-phosphate dianions (**I** and **II**) is the orientation of the phosphate group with respect to the pyranosyl ring (Fig. 2). The difference between values of the P–O–C–C torsion angles (P-1–O-1–C-1–C-2 −153.4(2)° and P-11–O-11–C-11–C-21 −130.1(3)°), which describe orientation of the phosphorus atom with respect to the sugar system, show that these conformational changes are not large and are probably induced by crystal-packing forces. Moreover, the phosphate groups have different arrangements of the terminal oxygen atoms with respect to the carbon atoms (Fig. 3). In molecule **I** one of the terminal oxygens—O-7—is in antiperiplanar with respect to the carbon atom, whereas two others oxygens—O-8, O-9—are synclinal. The conformations of the corresponding atoms in the other anion are unusual and one oxygen—O-71—is synperiplanar, the two others are anticlinal. The arrangement of the phosphate group found in **I** is characteristic for most mono-phosphate

Table 2. The puckering parameters for **I** and **II**

Structure	Ring	Q (Å)	Θ(°)	Φ (°)	Conformation
I	C-1–C-2–C-3–C-4–C-5–O-5	0.556(3)	−146.7(4)	177.3(3)	$^4C_1$
II	C-11–C-21–C-31–C-41–C-51–O-51	0.540(3)	48.7(4)	173.1(3)	$^4C_1$

Table 3. Selected bond lengths (Å), valence angles (°) and torsion angles (°)

Bond lengths			
P-1–O-7	1.518(3)	P-11–O-71	1.511(3)
P-1–O-8	1.517(2)	P-11–O-81	1.521(3)
P-1–O-9	1.523(3)	P-11–O-91	1.524(3)
P-1–O-1	1.630(3)	P-11–O-11	1.631(3)
O-1–C-1	1.422(4)	O-11–C-11	1.415(4)
O-2–C-2	1.429(4)	O-21–C-21	1.425(4)
O-3–C-3	1.434(4)	O-31–C-31	1.424(4)
O-4–C-4	1.425(4)	O-41–C-41	1.431(4)
O-5–C-1	1.409(4)	O-51–C-11	1.417(4)
O-5–C-5	1.441(3)	O-51–C-51	1.451(4)
O-6–C-6	1.433(4)	O-61–C-61	1.437(4)
C-1–C-2	1.522(4)	C-11–C-21	1.526(4)
C-2–C-3	1.527(4)	C-21–C-31	1.527(4)
C-3–C-4	1.520(4)	C-31–C-41	1.532(4)
C-4–C-5	1.537(4)	C-41–C-51	1.529(4)
C-5–C-6	1.520(4)	C-51–C-61	1.507(4)
Valence angles			
O-8–P-1–O-7	112.1(2)	O-81–P-11–O-71	114.1(2)
O-9–P-1–O-8	114.1(2)	O-91–P-11–O-81	112.9(2)
O-9–P-1–O-7	112.9(2)	O-91–P-11–O-71	112.3(2)
O-1–P-1–O-9	106.4(2)	O-11–P-11–O-91	104.8(2)
O-1–P-1–O-8	107.2(2)	O-11–P-11–O-81	103.7(2)
O-1–P-1–O-7	103.1(2)	O-11–P-11–O-71	108.1(2)
P-1–O-1–C-1	121.5(2)	P-11–O-11–C-11	121.9(2)
O-1–C-1–O-5	112.5(2)	O-11–C-11–O-51	110.3(2)
O-1–C-1–C-2	107.0(2)	O-11–C-11–C-21	109.3(2)
O-3–C-3–C-4	110.4(3)	O-31–C-31–C-41	108.6(3)
O-3–C-3–C-2	110.2(3)	O-31–C-31–C-21	110.6(2)
C-3–C-4–O-4	110.1(3)	C-31–C-41–O-41	107.1(3)
C-3–C-2–O-2	107.0(3)	C-31–C-21–O-21	111.6(3)
C-1–C-2–O-2	110.3(3)	C-11–C-21–O-21	108.7(2)
C-4–C-5–O-5	111.4(2)	C-41–C-51–O-51	109.0(2)
C-4–C-5–C-6	111.4(3)	C-41–C-51–C-61	113.3(2)
C-5–C-6–O-6	112.4(3)	C-51–C-61–O-61	110.1(3)
C-6–C-5–O-5	107.9(3)	C-61–C-51–O-51	106.8(2)
C-1–O-5–C-5	113.4(2)	C-11–O-51–C-51	115.3(2)
O-5–C-1–C-2	111.2(3)	O-51–C-11–C-21	112.1(3)
C-1–C-2–C-3	110.0(3)	C-11–C-21–C-31	111.7(3)
C-2–C-3–C-4	109.8(3)	C-21–C-31–C-41	112.0(3)
Torsion angles			
P-1–O-1–C-1–C-2	−153.4(2)	P-11–O-11–C-11–C-21	−130.1(3)
O-7–P-1–O-1–C-1	153.4(2)	O-71–P-11–O-11–C-11	1.4(3)
O-8–P-1–O-1–C-1	−88.1(3)	O-81–P-11–O-11–C-11	−120.1(3)
O-9–P-1–O-1–C-1	34.3(3)	O-91–P-11–O-11–C-11	121.3(3)
P-1–O-1–C-1–O-5	84.2(3)	P-11–O-11–C-11–O-51	106.2(3)
C-5–O-5–C-1–O-1	60.2(3)	C-51–O-51–C-11–O-11	65.6(3)
C-5–O-5–C-1–C-2	−59.8(3)	C-51–O-51–C-11–C-21	−56.5(3)
O-5–C-1–C-2–O-2	−60.0(3)	O-51–C-11–C-21–O-21	−75.0(3)
O-1–C-1–C-2–O-2	176.8(2)	O-11–C-11–C-21–O-21	162.4(3)
O-5–C-1–C-2–C-3	57.9(3)	O-51–C-11–C-21–C-31	48.6(3)
O-1–C-1–C-2–C-3	−65.3(3)	O-11–C-11–C-21–C-31	−74.1(3)
O-2–C-2–C-3–O-3	−56.2(3)	O-21–C-21–C-31–O-31	−47.5(4)
C-1–C-2–C-3–O-3	−176.1(3)	C-11–C-21–C-31–O-31	−169.4(2)
O-2–C-2–C-3–C-4	65.7(3)	O-21–C-21–C-31–C-41	73.8(3)
C-1–C-2–C-3–C-4	−54.2(3)	C-11–C-21–C-31–C-41	−48.1(3)
O-3–C-3–C-4–O-4	−66.2(3)	O-31–C-31–C-41–O-41	−66.0(3)
C-2–C-3–C-4–O-4	172.1(3)	C-21–C-31–C-41–O-41	171.6(3)
O-3–C-3–C-4–C-5	173.8(2)	O-31–C-31–C-41–C-51	175.1(3)
C-2–C-3–C-4–C-5	52.1(3)	C-21–C-31–C-41–C-51	52.7(3)
C-1–O-5–C-5–C-6	179.6(3)	C-11–O-51–C-51–C-61	−176.6(3)
C-1–O-5–C-5–C-4	57.1(3)	C-11–O-51–C-51–C-41	60.6(3)
O-4–C-4–C-5–O-5	−173.8(3)	O-41–C-41–C-51–O-51	−174.1(2)

Table 3 (*continued*)

C-3–C-4–C-5–O-5	−52.8(3)	C-31–C-41–C-51–O-51	−56.7(3)
O-4–C-4–C-5–C-6	65.7(3)	O-41–C-41–C-51–C-61	67.1(3)
C-3–C-4–C-5–C-6	−173.3(3)	C-31–C-41–C-51–C-61	−175.5(3)
O-5–C-5–C-6–O-6	61.3(3)	O-51–C-51–C-61–O-61	64.7(3)
C-4–C-5–C-6–O-6	−176.2(3)	C-41–C-51–C-61–O-61	−175.2(3)

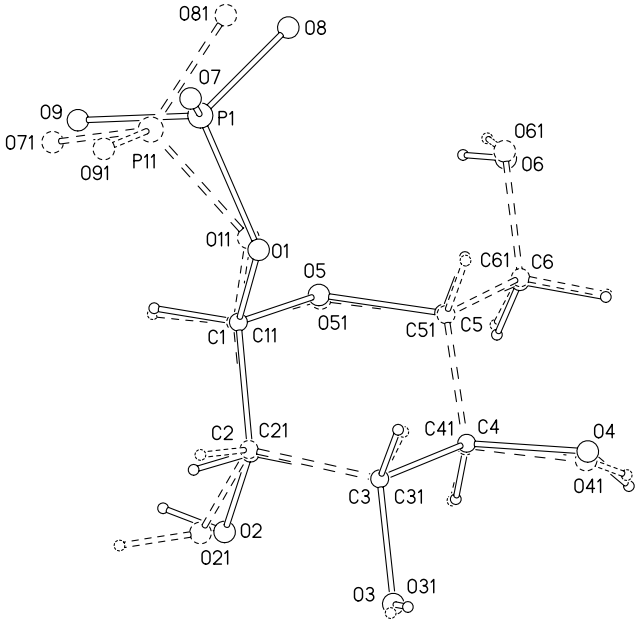

Figure 2. The overlapping scheme of the two independent anions **I** and **II** showing different orientation of the phosphate group.

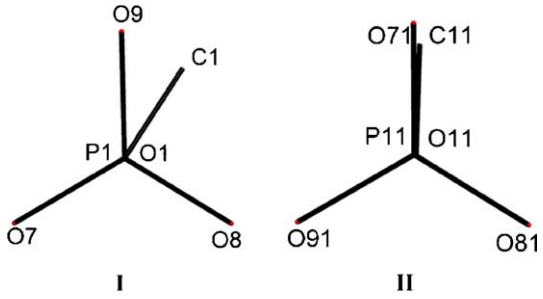

Figure 3. The Newman projections along P–$O_{(ester)}$ bonds.

molecules (428 structures),[14–16] whereas, the arrangement found in the other molecule was observed only in a few esters. Until now there have been published only four structures[16–20] in which the value of one torsion angle $O_{(terminal)}$–P–$O_{(ester)}$–C is less than 10°.[21] Such an orientation in **II** is probably caused by the extensive hydrogen-bond network and coordination to the potassium ions.

All water molecules and the hydroxyl O atoms are involved in the hydrogen-bond network (Table 4, Fig. 4).

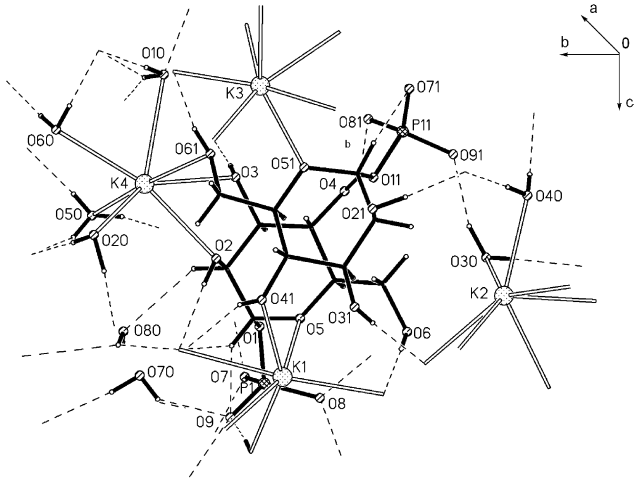

Figure 4. View of hydrogen bonds and coordination sphere of potassium ions.

Table 4. Geometry of hydrogen bonds and close C–H···O contacts (Å and °)

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
O-2–H-2···O-10(i)	0.81(4)	2.00(4)	2.811(3)	176(4)
O-3–H-3···O-9(ii)	0.74(4)	1.93(4)	2.667(3)	175(5)
O-4–H-4···O-81	0.84(4)	1.91(4)	2.688(3)	153(4)
O-6–H-6···O-81(i)	0.79(4)	1.89(4)	2.676(3)	174(4)
O-21–H-21···O-91(iii)	0.94(4)	1.73(4)	2.666(3)	172(4)
O-31–H-31···O-71(i)	0.69(4)	1.93(4)	2.615(3)	177(5)
O-41–H-41···O-8(iv)	0.64(4)	2.11(4)	2.697(3)	153(5)
O-61–H-61···O-8(v)	0.87(4)	1.83(4)	2.687(3)	169(4)
O-10–H-101···O-80(ii)	0.82(4)	1.87(4)	2.646(6)	156(4)
O-10–H-101···O-70(ii)	0.82(4)	2.14(4)	2.904(5)	154(4)
O-10–H-102···O-7(v)	0.75(4)	2.06(4)	2.811(3)	178(5)
O-20–H-201···O-7(iv)	1.11(5)	1.62(5)	2.719(3)	175(4)
O-20–H-202···O-20(vi)	0.70(4)	2.15(4)	2.810(5)	157(5)
O-30–H-301···O-71(vii)	0.75(4)	2.05(4)	2.802(5)	176(5)
O-30–H-302···O-91	0.93(4)	1.99(5)	2.888(3)	162(4)
O-40–H-402···O-91(iii)	0.81(4)	1.89(4)	2.695(3)	174(4)
O-40–H-401···O-21(vii)	0.68(4)	2.25(4)	2.927(3)	172(5)
O-50–H-501···O-9(viii)	0.81(5)	1.95(5)	2.751(4)	173(5)
O-50–H-502···O-50(ix)	0.92(9)	2.05(9)	2.869(6)	147(7)
O-50–H-503···O-20(vi)	0.89(10)	2.04(9)	2.833(4)	149(8)
O-60–H-60···O-7(viii)	0.88(8)	1.91(8)	2.789(3)	175(8)
O-70–H-701···O-9	0.86	2.14(5)	2.882(5)	145(7)
O-70–H-702···O-9(ix)	0.86	2.07(5)	2.925(5)	169(8)
O-80–H-802···O-7(ix)	0.86	2.56(8)	2.850(6)	101(6)
O-80– H-802···O–10(i)	0.86	2.12(7)	2.646(6)	119(7)
C-1–H-1A···O-10(i)	1.00	2.64	3.375(4)	130
C-1–H-1A···O-9	1.00	2.43	2.923(4)	110
C-2–H-2A···O-80	1.00	2.63	3.209(6)	117
C-11–H-11A···O-71	1.00	2.29	2.859(4)	115

Symmetry codes: (i) $x,y,z+1$; (ii) $x,y,z-1$; (iii) $x+1/2,-y+1/2,-z$; (iv) $x+1,y,z$; (v) $x+1,y,z-1$; (vi) $-x+2,-y+1,z$; (vii) $x-1/2,-y+1/2,-z$; (viii) $-x+1,-y+1,z-1$; (ix) $-x+1,-y+1,z$.

Table 5. Shortest K···O and K···K distances (Å)

K-1···O-3(i)	2.784(2)	K-3···O-8(v)	2.627(2)
K-1···O-5	2.843(2)	K-3···O-31(ii)	2.820(2)
K-1···O-10(i)	2.858(3)	K-3···O-40(iii)	2.725(3)
K-1···O-41	2.734(3)	K-3···O-41(ii)	3.124(3)
K-1···O-61(i)	2.801(2)	K-3···O-51	2.702(2)
K-1···O-81(i)	2.714(2)	K-4···O-2	2.734(3)
K-2···O-6(x)	2.824(2)	K-4···O-3	2.914(2)
K-2···O-21(xi)	2.753(2)	K-4···O-10	2.950(3)
K-2···O-30	2.824(3)	K-4···O-20	2.796(3)
K-2···O-30(x)	3.045(3)	K-4···O-50	2.790(3)
K-2···O-31(xi)	2.788(2)	K-4···O-60	2.766(2)
K-2···O-40	2.727(3)	K-4···O-61	2.796(2)
K-2···O-71(i)	2.769(2)	K-1···K-3(i)	4.414(2)
K-3···O-4(iv)	2.684(2)	K-1···K-4(i)	3.904(2)
K-3···O-6(v)	2.698(2)	K-2···K-3(vii)	3.697(2)

Symmetry transformations used to generate equivalent atoms: (i) $x,y,z+1$; (ii) $x,y,z-1$; (iii) $x+1/2,-y+1/2,-z$; (iv) $x+1,y,z$; (v) $x+1,y,z-1$; (vii) $x-1/2,-y+1/2,-z$; (x) $x+1/2,-y+1/2,-z+1$; (xi) $x-1/2,-y+1/2,-z+1$.

There are also four C–H···O short contacts found in the crystal structure. Two of them are intramolecular—C-11–H-11A···O-71 and C-1–H-1A···O-9 (Table 4). In the packing arrangement, water molecules define layers lying perpendicular to the *b*-axis. These alternate with layers in which the mannose phosphate molecules are packed together (Figs. 4 and 5).

The potassium cations are six- (K1) and seven- (K2, K3, K4) coordinate (Fig. 4). They are coordinated to oxygen atoms of water molecules, phosphate groups, hydroxyl groups and to endocyclic O atoms of the sugar rings. The K···O distances are characteristic for other potassium salts[22] (Table 5). In the packing arrangement potassium ions are located in channels extending along *c*-axis (Fig. 5).

3. Experimental

Crystals suitable for X-ray studies were obtained by slow diffusion of EtOH into a dilute water solution of the compound. The preliminary oscillation and Weissenberg photographs determined the approximate unit-cell dimensions. The intensities data collections were carried out on a KUMA KM4 κ-axis diffractometer with a CCD camera and an Oxford Cryosystem device. All data were corrected for Lorentz and polarization effects. Data reduction and analysis were carried out with the Kuma Diffraction programs. The structure was solved by direct methods and refined by the full-matrix least-squares method on F^2 data using the SHELXTL (version 5.1) program.[23] The absolute configuration was defined basing on the known stereochemistry of D-mannose. Carbon-bonded hydrogen atoms were included in calculated positions and refined in the riding mode. All other H-atoms were located on Fourier difference maps. All H-atoms were included with temperature factors 20% greater than U_{eq} of the parent atom. Lengths of the O–H bonds in O(70) and O(80) water molecules were assumed as 0.86 Å by means of DFIX instruction. The final atomic parameters are given in Table 6. The refinement process showed that occupancy factors for the O-60 atom (one of water molecules) is 0.5 as well as that one water molecule is disordered over two positions O-70 and O-80.

Table 6. Atomic coordinates and equivalent isotropic displacement parameters

$$U_{eq} = 1/3 \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j$$

Atom	*x*	*y*	*z*	U_{eq}
P-1	0.2544(1)	0.43503(2)	0.5603(1)	0.011(1)
O-1	0.3479(2)	0.42809(5)	0.3761(3)	0.013(1)
O-2	0.7255(2)	0.42241(5)	0.2032(3)	0.015(1)
O-3	0.5729(2)	0.41954(5)	−0.1188(3)	0.014(1)
O-4	0.4300(2)	0.36031(5)	−0.0516(3)	0.014(1)
O-5	0.5174(2)	0.38695(5)	0.4080(3)	0.012(1)
O-6	0.4126(2)	0.32570(5)	0.4813(3)	0.013(1)
O-7	0.1357(2)	0.45765(5)	0.4984(3)	0.015(1)
O-8	0.1883(2)	0.40456(5)	0.6224(3)	0.014(1)
O-9	0.3640(2)	0.44928(5)	0.6933(3)	0.016(1)
C-1	0.5000(3)	0.41902(7)	0.3813(4)	0.011(1)
C-2	0.5698(3)	0.42926(7)	0.2040(4)	0.012(1)
C-3	0.5003(3)	0.41150(7)	0.0471(4)	0.012(1)
C-4	0.5122(3)	0.37691(7)	0.0813(4)	0.011(1)
C-5	0.4501(3)	0.36848(7)	0.2681(4)	0.011(1)
C-6	0.4779(3)	0.33465(7)	0.3127(4)	0.014(1)
P-11	0.6905(1)	0.29776(2)	−0.1750(1)	0.010(1)
O-11	0.7804(2)	0.31125(5)	−0.0007(3)	0.014(1)
O-21	1.1236(2)	0.28385(5)	0.1964(3)	0.014(1)
O-31	1.0157(2)	0.30849(5)	0.5154(3)	0.012(1)
O-41	0.9822(3)	0.37211(5)	0.4374(3)	0.015(1)
O-51	1.0059(2)	0.33749(5)	−0.0154(3)	0.012(1)
O-61	0.9846(2)	0.40064(5)	−0.1131(3)	0.015(1)
O-71	0.8019(2)	0.28249(5)	−0.2993(3)	0.013(1)
O-81	0.6159(2)	0.32625(5)	−0.2549(3)	0.014(1)
O-91	0.5797(2)	0.27472(5)	−0.0966(3)	0.014(1)
C-11	0.9367(3)	0.30850(7)	0.0155(4)	0.011(1)
C-21	0.9750(3)	0.29533(7)	0.2008(4)	0.012(1)
C-31	0.9541(3)	0.31932(7)	0.3499(4)	0.011(1)
C-41	1.0272(3)	0.35031(7)	0.3025(4)	0.010(1)
C-51	0.9734(3)	0.36125(7)	0.1174(4)	0.013(1)
C-61	1.0493(3)	0.39040(7)	0.0539(4)	0.013(1)
K-1	0.7485(2)	0.38109(1)	0.6678(1)	0.014(1)
K-2	0.7605(1)	0.23115(1)	0.4829(1)	0.014(1)
K-3	1.2084(1)	0.34626(2)	−0.2802(1)	0.013(1)
K-4	0.8387(1)	0.45735(2)	−0.0720(1)	0.018(1)
O-10	0.8354(3)	0.44092(6)	−0.4584(3)	0.019(1)
O-20	1.0815(3)	0.47224(6)	0.1476(4)	0.024(1)
O-30	0.5347(3)	0.26051(6)	0.2804(3)	0.019(1)
O-40	0.7918(3)	0.20935(6)	0.1395(3)	0.016(1)
O-50	0.6540(3)	0.50873(6)	−0.0285(4)	0.025(1)
O-60	1	0.5	−0.2696(5)	0.017(1)
O-70	0.6026(5)	0.48746(1)	0.5588(7)	0.019(1)
O-80	0.6893(5)	0.48932(12)	0.4136(7)	0.023(1)

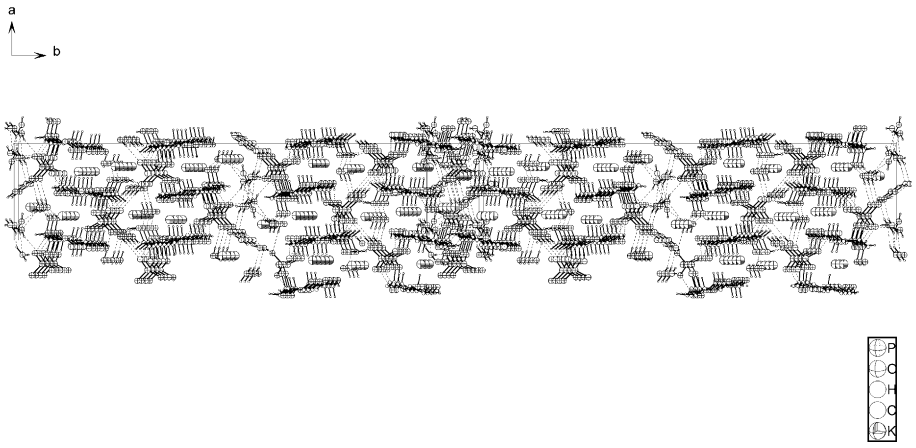

Figure 5. The packing diagram showing potassium channels along *c*-axis (stereo view with pictures' distance 12 cm and stereo angle 6°).

4. Supplementary data

Cambridge Crystallographic Data Center (CCDC) contains the supplementary crystallographic data for this letter: CCDC 270606.

These data may be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033, e-mail: deposit@ccdc.cam.ac.uk).

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