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Multicomponent Polyanions

VI. The Molecular and Crystal Structure of $Na_4H_2Mo_5P_2O_{23}(H_2O)_{10}$, a Compound Containing Sodium-coordinated Dihydrogenpentamolybdodiphosphate Anions

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The crystal structure of $Na_4H_2Mo_5P_2O_{23}(H_2O)_{10}$ has been determined from three-dimensional X-ray diffraction data collected with a PAILRED diffractometer using Mo$K\alpha$-radiation. The cell dimensions of the monoclinic ($P2_1/n$) unit cell are $a = 26.388(2)$ Å, $b = 13.661(1)$ Å, $c = 8.041(1)$ Å, and $\beta = 91.37(1)°$, and it contains four formula units. The structure consists of $H_2Mo_5P_2O_{23}^{4-}$-groups linked together by direct sodium bridges (O–Na–O) in the y- and z-directions forming infinite layers parallel to the yz-plane. The layers are held together by O–Na–H_2O–Na–O linkages. Each sodium ion is surrounded by six oxygen atoms (water oxygens and group oxygens), which form an octahedron. The structure has been refined by least squares methods using anisotropic vibrational parameters and the final R-value is 0.053, based on 3897 independent reflexions.

In emf-investigations of aqueous equilibria involving H^+, MoO_4^{2-} and HPO_4^{2-}, the complexes $(H^+)_8(MoO_4^{2-})_5(HPO_4^{2-})_2^{6-}$, $(H^+)_9(MoO_4^{2-})_5(HPO_4^{2-})_2^{5-}$, and $(H^+)_{10}(MoO_4^{2-})_5(HPO_4^{2-})_2^{4-}$ have been reported.[1] In connection with these studies different crystalline phases have been obtained. X-Ray diffraction investigations have been carried out with some of these.[2] The crystal structure of $Na_6Mo_5P_2O_{23}(H_2O)_{13}$, corresponding to the complex $(H^+)_8(MoO_4^{2-})_5(HPO_4^{2-})_2^{6-}$, has been completely determined.[2]

The present work presents the crystal data and structure of $Na_4H_2Mo_5P_2O_{23}(H_2O)_{10}$, the phase which corresponds to the complex $(H^+)_{10}(MoO_4^{2-})_5(HPO_4^{2-})_2^{4-}$. For brevity, $Na_6Mo_5P_2O_{23}(H_2O)_{13}$ and $Na_4H_2Mo_5P_2O_{23}(H_2O)_{10}$ will be referred to in the text as (8,5,2) and (10, 5,2), respectively.

EXPERIMENTAL

Crystal preparation and analyses. In a typical preparation of the crystals, $Na_2MoO_4.2H_2O$ and $NaH_2PO_4.2H_2O$ were dissolved in concentrated $HClO_4$. The concentrations were $[MoO_4^{2-}]_{tot} = 1.60$ M, $[HPO_4^{2-}]_{tot} = 0.64$ M, and $[HClO_4]_{tot} = 2.57$ M.

After a few days (sometimes weeks) of evaporation at room temperature colourless acicular crystals were formed. The crystals were not stable in air, and during the X-ray exposures they were sealed together with part of the mother liquid in a capillary of Lindeman glass. The contents of Na, Mo, and P were determined by elemental analyses (carried out at the Department of Analytical Chemistry, University of Umeå). (Found: Na 7.9; Mo 41.0; P 5.2. Calc.: Na 7.8; Mo 40.5; P 5.2.) The water content of the crystal was investigated by Karl Fischer titration and a value of 16.2 % (calc. 15.2 %) was found. Thermobalance analysis confirmed the amount of water.

Crystal data and space group. Rotation photographs around [100], [010] and [001] and the corresponding Weissenberg photographs (zero, first and second layer lines) taken with Cu$K\alpha$-radiation ($\lambda = 1.5418$ Å) revealed that the crystals were monoclinic. This was confirmed from precession photographs.

Accurate unit cell dimensions were determined with a Hägg-Guinier camera with Si as internal standard. The parameters and their corresponding standard deviations are: $a = 26.388 \pm 0.002$ Å, $b = 13.661 \pm 0.001$ Å, $c = 8.041 \pm 0.001$ Å, $\beta = 91.37° \pm 0.01°$, $V = 2897.8$ Å^3.

The calculated density with $Z = 4$ is 2.71 g cm^{-3}, which is in agreement with the observed density of 2.71 ± 0.01 g cm^{-3} determined by flotation in a bromoform-carbon tetrachloride solution. Systematic extinctions were found for $h0l$, $h+l = 2n+1$ and $0k0$, $k = 2n+1$ and the space group was uniquely determined as $P2_1/n$ ($P2_1/c$, No. 14 in Ref. 3, in a different orientation).

Collection and reduction of intensity data. Three-dimensional intensity data were at 25°C collected with a Philips PAILRED linear diffractometer using Mo$K\alpha$-radiation reflected off the (200) plane of a LiF-monochromator crystal ($\lambda = 0.7107$ Å). A crystal of approximate dimensions $0.07 \times 0.20 \times 0.26$ mm was mounted and rotated along the c-axis (parallel to the 0.26 mm-edge of the crystal). A total of 6834 reflexions of the type hkl and $\bar{h}kl$ from the layers $hk0 - hk7$ were scanned up to a limit of $\sin\theta \approx 0.55$. The integrated reflexions were corrected for background in the usual way,[4] and since the zero level reflexions $hk0$ and $\bar{h}k0$ were equivalent within experimental error, the $hk0$ reflexions were used. Reflexions with a relative statistical error of $\Delta I_o/I_o$ greater than 0.3 were omitted leaving a remaining data set of 4538 unique observed reflexions.

During the refinement it became obvious that some reflexions of high $\sin\theta$-values showed noticeable differences between the observed and calculated structure factor values. A thorough investigation including comparison with films and analyses of the reflexion profiles on the charts showed that extra peaks had occurred. Since the a-axis is 26.388 Å, these were possibly caused by strong reflexions of about the same $\sin\theta$. 104 reflexions showing this effect were deleted from the material. In addition the 537 reflexions from the $hk7$ layer were omitted since no film for comparison was available. The refinements were then based on the remaining 3897 reflexions. The intensities were corrected for Lorentz and polarization effects and absorption correction was applied with a $4 \times 10 \times 12$ grid ($\mu = 23.65$ cm^{-1}).

Computer programs used. The computer programs for Lorentz, polarization and absorption corrections were originally written by P. Coppens, L. Leiserowitz and D. Rabinovich. Fourier summations and calculation of distances and angles were performed with programs originally written by A. Zalkin. A modified version of a program written by Gantzel, Sparks and Trueblood was used in the least squares refinements of the structural parameters (full-matrix) and for block-diagonal refinements the program BLOCK written by Ove Lindgren, University of Gothenburg, was used. The stereoscopic figures were produced by the program ORTEP.[5] The computations were carried out with a CDC 3200 computer in Umeå and an IBM 360/65 computer in Gothenburg.

Crystal data:

$Na_4H_2Mo_5P_2O_{23}(H_2O)_{10}$ F. W. = 1183.8

Monoclinic $P2_1/n$, all atoms in 4(e): $\pm(x, y, z; \frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z)$

$a = 26.388(2)$ Å
$b = 13.661(1)$ Å
$c = 8.041(1)$ Å
$\beta = 91.37(1)°$
$V = 2897.8$ Å^3

$Z = 4$
$D_x = 2.71$ g cm^{-3}
$D_m = 2.71 \pm 0.01$ g cm^{-3}
$\mu = 23.63$ cm^{-1}

STRUCTURE DETERMINATION AND REFINEMENT

The space group implies that symmetry vectors on a Harker line $(\frac{1}{2},2y+\frac{1}{2},\frac{1}{2})$ and in a Harker plane $(2x+\frac{1}{2},\frac{1}{2},2z+\frac{1}{2})$ should be found in a Patterson synthesis. The computed three-dimensional synthesis [normalized to $P(0,0,0)=999$] contained three peaks on the line and eleven in the plane, all of them of height 130 – 160. In addition a peak of height ≈ 300 was found at (0.5,0,0.3). Two of the Harker line vectors could be shown to be doublets, and in combination with $(2x,2y,2z)$ vectors four molybdenum atoms were located. The coordinates of the fifth atom were obtained from cross vectors. The (0.5,0,0.3) vector was explained as a multiple cross vector between different formula units.

A Fourier synthesis based on the molybdenum atoms gave a conventional R-value of 0.338. It confirmed the positions of the molybdenum atoms and also gave the positions of phosphorus and oxygen atoms belonging to the $H_2Mo_5P_2O_{23}^{4-}$-group. In a second Fourier synthesis four sodium atoms and ten water oxygen atoms could be located, while the R-value decreased to 0.243. The positional parameters and isotropic temperature factors for the 44 non-hydrogen atoms in the asymmetric unit were refined by full-matrix least squares methods. The function minimized was $\sum\omega(|F_o|-|F_c|)^2$ and the residual $R=\sum||F_o|-|F_c||/\sum|F_o|$ was reduced from 0.243 to 0.073 in five iterations. The refinements were then continued with anisotropic vibrational parameters using a block-diagonal matrix approximation which resulted in a final R-value of 0.053.

The atomic scattering factors used for Mo^{3+} were those given by Cromer and Waber,[6] for P those given by Hanson, Herman, Lea and Skillman,[7] and for Na^+, O^-, and O the values in International Tables.[8] To obtain electroneutrality $f(O)$ was used for water oxygen atoms and $f(O^-)$ for the remainder. Account was taken of the real part of the dispersion correction.[8]

A weighting scheme according to Cruickshank [9] was applied: $\omega=1/(a+|F_o|+c|F_o|^2+d|F_o|^3)$ where the values of the constants were $a=60$, $c=0.008$, and $d=0$.

A difference Fourier synthesis based on 2809 reflexions with a maximum of sin $\theta\approx 0.45$ was searched for possible hydrogen atom peaks around the $H_2Mo_5P_2O_{23}^{4-}$-group. Two peaks at acceptable oxygen-hydrogen distances were found and the positional parameters were included in a block-diagonal least squares refinement (scattering factors for H from Stewart *et al.*[10]). The decrease in R-value was significant on the 10 %-level according to the Hamilton test as approximated by Pawley.[11] However, since there were higher peaks in the difference Fourier for which no explanations were found, no values of hydrogen atom parameters are given. The sites for the tested peaks are identical with the hydrogen atom positions as discussed later in the text.

Final atomic coordinates and vibrational parameters and corresponding standard deviations are given in Tables 1 and 2, and a comparison of the observed and calculated structure factors is given in Table 3.

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

The structure is built up from $H_2Mo_5P_2O_{23}^{4-}$-anions, Na^+-ions and H_2O molecules. The Mo atoms in the $H_2Mo_5P_2O_{23}^{4-}$-groups form pentagons the

Table 1. The fractional atomic coordinates and in parentheses their estimated standard deviations (referring to the last decimal place given).
For the oxygen atoms O(*ij*) or OP(*ij*) the index means that the atom is bonded to the molybdenum atoms *i* and *j*. Aq(*ij*) is a water oxygen bonded to the sodium ions *i* and *j*.

	x	*y*	*z*
Mo1	0.23748(3)	0.25607(7)	0.2772 (1)
Mo2	0.16157(3)	0.44947(6)	0.3501 (1)
Mo3	0.03942(3)	0.37272(6)	0.3485 (1)
Mo4	0.04162(3)	0.12885(6)	0.1540 (1)
Mo5	0.16453(3)	0.05712(6)	0.1832 (1)
P1	0.1257(1)	0.2143(2)	0.4824 (4)
P2	0.1269(1)	0.2913(2)	0.0398 (4)
O1(1)	0.2765(3)	0.2726(6)	0.4481(11)
O2(1)	0.2792(3)	0.2421(6)	0.1211(11)
O(12)	0.2148(3)	0.3869(5)	0.2307(11)
O(15)	0.2161(3)	0.1229(5)	0.3119(10)
OP(12)	0.1696(3)	0.2849(5)	0.4470 (9)
OP(15)	0.1713(2)	0.2230(5)	0.0825(10)
O1(2)	0.1916(3)	0.4860(6)	0.5294(11)
O2(2)	0.1577(3)	0.5514(5)	0.2298(11)
O(23)	0.0933(2)	0.4515(5)	0.4382(10)
OP(23)	0.1127(3)	0.3556(5)	0.1897 (9)
O1(3)	−0.0041(3)	0.3836(6)	0.5002(10)
O2(3)	0.0154(3)	0.4493(5)	0.1934(10)
OP(3)	0.0783(3)	0.2677(5)	0.5301(10)
O(34)	0.2172(3)	0.2509(5)	0.2497(10)
O1(4)	0.1719(3)	0.0525(6)	0.3013(12)
O2(4)	−0.0006(3)	0.1176(6)	−0.0082(12)
OP(4)	0.0800(2)	0.2369(5)	−0.0170(10)
O(45)	0.0964(3)	0.0522(5)	0.0783(10)
OP(45)	0.1134(3)	0.1488(5)	0.3279(10)
O1(5)	0.1601(3)	−0.0441(6)	0.3053(13)
O2(5)	0.1955(3)	0.0190(7)	0.0104(12)
OP1	0.1464(3)	0.1466(6)	0.6255(10)
OP2	0.1468(3)	0.3600(5)	−0.0999(10)
Na1	0.5239(2)	0.2485(4)	0.2542 (7)
Na2	0.3678(3)	0.1989(5)	0.3726 (9)
Na3	0.3225(2)	0.2003(5)	−0.1183 (8)
Na4	0.2599(2)	0.4092(5)	0.6927 (8)
Aq(1)	0.4715(4)	0.3517(6)	0.0862(13)
Aq(12)	0.4640(4)	0.1493(7)	0.4056(13)
Aq(2)	0.3946(5)	0.3365(9)	0.4890(23)
Aq1(23)	0.3966(3)	0.1998(8)	0.0651(13)
Aq2(23)	0.3468(4)	0.1202(7)	0.6404(13)
Aq1(34)	0.2391(4)	0.2381(10)	0.7848(13)
Aq2(34)	0.3386(4)	0.3754(9)	0.8427(20)
Aq(4)	0.2391(3)	0.4996(6)	0.9402(12)
Aq1	0.0847(3)	0.0166(7)	0.7479(11)
Aq2	0.0811(3)	0.4796(7)	−0.2383(12)

Table 2. The final anisotropic thermal parameters ($\times 10^4$) and their estimated standard deviations ($\times 10^4$) in parentheses. The parameters are calculated according to the formula exp $[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+hk\beta_{12}+hl\beta_{13}+kl\beta_{23})]$

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Mo1	6(0)	28(0)	70(2)	4(0)	10(1)	10(1)
Mo2	6(0)	21(0)	70(2)	−2(0)	8(1)	−6(1)
Mo3	6(0)	20(0)	75(2)	1(0)	10(1)	−11(1)
Mo4	6(0)	20(0)	79(2)	−2(0)	5(1)	−9(1)
Mo5	7(0)	25(0)	87(2)	8(0)	3(1)	−9(1)
P1	6(0)	22(1)	55(6)	0(1)	7(2)	6(3)
P2	6(0)	21(1)	57(6)	0(1)	5(2)	4(3)
O1(1)	8(1)	40(5)	119(19)	1(4)	−1(6)	30(13)
O2(1)	9(1)	44(5)	73(17)	8(4)	19(6)	6(13)
O(12)	6(1)	22(3)	92(17)	1(3)	17(5)	12(11)
O(15)	7(1)	27(4)	59(16)	8(3)	0(5)	21(11)
OP(12)	9(1)	25(3)	29(15)	−3(3)	14(5)	−7(10)
OP(15)	6(1)	24(3)	67(16)	10(3)	4(5)	−4(10)
O1(2)	7(1)	46(5)	78(17)	−8(4)	0(6)	−53(13)
O2(2)	12(1)	25(4)	88(18)	4(3)	22(6)	24(12)
O(23)	5(1)	19(3)	94(16)	0(3)	6(5)	−27(10)
OP(23)	7(1)	19(3)	50(15)	3(3)	17(5)	−9(9)
O1(3)	7(1)	35(4)	61(16)	0(3)	24(6)	−45(11)
O2(3)	8(1)	25(4)	81(17)	6(3)	7(6)	−14(11)
OP(3)	7(1)	22(3)	82(17)	−1(3)	21(5)	−4(10)
O(34)	8(1)	24(3)	74(16)	6(3)	16(5)	−33(11)
O1(4)	11(1)	30(4)	114(19)	−8(4)	6(7)	2(13)
O2(4)	9(1)	28(4)	135(20)	−3(3)	5(6)	−39(13)
OP(4)	6(1)	22(3)	74(16)	−1(3)	−8(5)	−3(10)
O(45)	8(1)	23(3)	71(17)	6(3)	5(5)	−16(11)
OP(45)	8(1)	27(4)	65(16)	4(3)	7(5)	−26(11)
O1(5)	11(1)	31(4)	153(21)	4(4)	−6(7)	22(14)
O2(5)	10(1)	49(5)	124(20)	18(4)	10(7)	−42(15)
OP1	9(1)	34(4)	49(16)	3(3)	−1(5)	25(11)
OP2	9(1)	32(4)	58(16)	0(3)	7(6)	32(11)
Na1	9(1)	73(4)	91(11)	−3(3)	4(4)	5(9)
Na2	20(1)	60(3)	215(15)	−24(3)	35(6)	−101(12)
Na3	11(1)	78(4)	129(12)	10(3)	5(4)	−41(11)
Na4	19(1)	85(4)	128(14)	28(4)	−5(5)	18(12)
Aq(1)	15(1)	33(4)	146(22)	2(4)	17(8)	19(14)
Aq(12)	15(1)	49(5)	134(22)	2(5)	7(8)	13(16)
Aq(2)	16(2)	49(7)	519(49)	5(6)	−18(15)	−82(28)
Aq1(23)	10(1)	60(6)	204(24)	3(5)	14(8)	39(19)
Aq2(23)	15(1)	44(5)	140(21)	4(5)	9(8)	−1(15)
Aq1(34)	10(1)	120(10)	111(24)	2(6)	−7(8)	−36(22)
Aq2(34)	15(2)	76(8)	301(34)	3(6)	6(12)	125(28)
Aq(4)	12(1)	44(5)	111(20)	10(4)	6(7)	−5(14)
Aq1	13(1)	54(5)	106(20)	21(5)	15(7)	16(15)
Aq2	12(1)	50(5)	86(19)	−20(4)	5(7)	−7(14)

planes of which are approximately parallel to the xy-plane. Three of the Na^+-ions act as links in O−Na−O-bridges between adjacent groups and two symmetry-related zigzag chains parallel to the y-axis are formed this way (Fig. 1). The difference in z between the chains is about 4 Å. The fourth Na^+-ion

Table 3. Observed and calculated structure factors. The columns are h, $|F_o|$, and F_c, respectively.

H 17 0		H 9 0		2 243 -232		8 120 113		20 64 -63		-17 89 86	
10 58 -65		28 30 -31		1 51 -53		10 372 -372		19 75 76		-19 31 -31	
6 104 -105		26 40 -39				12 138 133		17 37 -34		-23 63 -60	
4 75 -77		24 83 81		H 4 0		14 276 -277		15 100 -103		-24 110 -104	
		22 31 -27		0 63 59		16 277 -268		14 27 33		-27 75 -67	
H 16 0		20 130 133		1 50 48		18 97 96		13 49 -49			
0 143 151		19 32 36		2 421 -410		20 42 -36		10 41 45		H 10 1	
1 33 -37		18 60 52		4 55 -58		24 238 225		9 130 -134		-27 87 -84	
4 79 83		16 107 108		5 25 -27		26 140 128		8 30 -36		-23 51 48	
8 38 -40		15 35 37		6 163 -157		28 80 -74		7 35 39		-21 40 -40	
10 86 -95		14 58 -57		8 87 98		30 109 99		6 25 -20		-20 80 -82	
14 70 -75		10 100 -101		9 20 20		34 84 -78		5 46 44		-19 46 -45	
		8 54 -52		10 98 101				3 27 -18		-18 72 -72	
H 15 0		6 176 -178		12 328 338		H 17 1		2 74 -70		-17 104 102	
18 54 -56		4 109 -107		14 82 93		7 35 36		1 148 145		-16 58 -58	
16 76 -79		2 169 -165		16 106 115		6 32 35		0 44 -47		-14 40 -38	
14 103 112		1 24 -26		18 43 -45		3 74 -76		-1 148 144		-13 113 -110	
12 27 -30				20 148 -150		1 48 -53		-2 31 -27		-12 60 58	
8 74 77		H 8 0		22 102 -100		0 80 92		-6 38 -41		-11 87 85	
6 100 105		0 223 206		24 102 -99		-3 44 -48		-7 65 60		-10 50 -47	
2 50 53		2 145 143		26 89 -85		-4 32 -34		-8 34 31		-9 82 -83	
		3 64 69		28 174 -167		-5 38 -39		-9 141 -140		-8 98 93	
H 14 0		4 382 377		30 30 26		-7 45 48		-12 42 39		-7 52 -47	
0 26 29		5 97 -99				-10 49 -48		-13 63 -61		-6 130 126	
1 28 28		6 226 -228		H 3 0				-15 64 -64		-4 96 95	
2 49 47		7 40 40		32 131 -122		H 16 1		-16 30 33		-1 211 -202	
3 28 -27		8 28 25		29 42 36		-10 47 55		-17 43 -44		0 62 64	
4 78 -81		10 83 -86		28 83 -76		-9 60 60		-19 79 80		1 215 210	
5 37 34		12 221 -227		24 56 -54		-7 87 88		-21 55 -61		2 76 -79	
6 40 42		13 27 26		23 24 20		-6 54 61		-22 42 -41		3 46 -45	
7 29 -25		14 87 -88		22 135 131		-5 44 55		-23 70 68		4 68 -64	
12 70 -74		18 128 -133		20 115 -114		-1 86 89				6 116 -118	
14 38 -38		19 27 24		19 38 -38		0 42 -40		H 12 1		7 81 83	
		20 55 52		18 308 310		1 71 -73		-23 70 72		8 29 -36	
H 13 0		22 150 150		16 88 90		2 72 79		-22 40 40		9 86 97	
20 45 44		26 125 124		14 22 15		4 42 -45		-19 63 61		11 146 -159	
18 106 -108		28 110 109		13 40 -41		5 70 -74		-18 54 57		13 173 185	
16 95 -95		30 29 -25		12 75 -77		6 46 -47		-17 122 121		14 26 -28	
9 30 -27				10 105 110		7 62 -63		-15 35 -33		16 36 38	
8 185 190		H 7 0		8 190 -213		9 73 -75		-14 67 -64		17 99 -103	
7 37 42		30 116 112		7 26 28		12 34 -37		-10 64 65		18 77 77	
3 39 -42		26 25 -21		6 149 -130		13 27 -26		-9 86 -87		20 58 53	
2 175 174		24 28 -23		3 38 -31		14 37 38		-8 105 -99		21 31 31	
1 45 43		20 191 -193		2 220 -212				-7 165 -163		23 73 -73	
		18 28 27				H 15 1		-4 32 -37		24 42 40	
H 12 0		16 91 -91		H 2 0		14 80 -83		-3 152 -151		25 30 35	
0 245 -238		14 73 -75		0 121 -124		13 35 37		-2 31 -30			
2 123 -125		10 205 212		2 33 30		9 66 -69		-1 45 -45		H 9 1	
4 96 98		8 25 -33		3 44 -49		8 47 -50		1 79 79		29 45 -42	
6 165 -171		6 195 200		4 161 -161		5 65 67		2 64 62		28 36 38	
7 37 40		5 29 -29		5 58 65		4 54 56		3 112 115		26 48 51	
8 72 71		4 184 185		6 284 296		3 26 -27		6 82 83		25 98 -97	
10 109 114		2 37 -32		7 50 -55		2 29 27		7 172 175		22 53 53	
12 84 88		1 35 36		8 261 -265		1 75 77		9 43 45		21 74 -75	
14 55 52				9 36 32		-1 94 98		10 48 -48		17 32 -34	
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-6 100 103	11 178 176	-6 29 36
-7 133 -136	10 158 152	-2 172 172
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-12 85 -87	-5 111 -105	5 45 -48
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-15 74 81	-8 32 25	10 57 57
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	-25 27 29	-1 71 67
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-24 133 -129	-26 52 -53	-15 74 -76
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-19 51 -52	-10 212 212	-18 50 -48

Table 3. Continued.

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Table 3. Continued.

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Table 3. Continued.

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Table 3. Continued.

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-6	104	106	-16	60	65	-17	64	66	-19	30	30	-28	78	-88	-14	78	-74
-7	65	63	-15	55	-57	-15	49	46	-18	43	-44	-27	37	41	-12	37	-32
-8	48	-46	-14	123	-126	-13	27	21	-16	95	101	-26	57	66	-10	185	-193
-9	36	31	-12	92	-92	-12	64	-65	-15	28	-24	-25	52	59	-8	23	24
-10	88	92	-10	23	22	-11	62	63	-14	65	74	-24	52	-61	-6	129	129
-11	40	39	-9	50	-42	-10	62	63	-13	34	37	-23	57	63	4	15	-13
-14	40	-38	-8	76	-71	-9	52	57	-12	84	81	-22	24	-28	6	188	184
-16	46	-48	-6	60	-53	-8	20	-17	-11	33	33	-18	79	90	8	173	-169
-17	38	-35	-5	68	66	-7	36	29	-10	26	29	-16	125	-142	10	48	-45
-18	35	28	-4	104	98	-6	26	-25	-9	46	-50	-14	34	37	12	82	-80
-21	33	-32	-2	112	103	-5	21	-25	-6	33	32	-13	104	-113	14	61	-52
			-1	23	-23	-4	70	71	-5	60	58	-12	58	61	16	92	-83
	H 10	6	2	185	178	-3	67	-58	-4	165	-151	-11	69	-74	18	170	152
-25	31	30	3	28	23	-2	34	-31	-3	51	46	-10	106	-112	20	69	-63
-24	57	-53	6	46	-46	-1	44	-45	-2	107	-98	-8	48	51	22	67	58
-23	74	71	12	195	-190	1	20	-18	-1	87	-76	-7	21	15	24	152	125
-22	86	90	14	30	30	3	54	-51	0	194	-178	-6	142	148	26	86	71
-20	72	-77	15	34	-36	4	51	53	1	36	-35	-4	40	-40	30	90	70
-16	69	66	16	47	-47	5	53	-51	2	95	-92	-3	41	31	32	48	-38
-14	23	-15	19	28	27	6	64	-67	3	68	68	-1	148	133			
-13	80	-85	20	57	54	7	73	73	4	120	-125	0	142	129			
-12	56	-57	21	27	26	8	77	83	5	33	37	1	98	100			
-11	28	-28	22	98	90	9	38	43	6	56	60	2	154	-164			
-10	99	101	23	47	-41	10	31	-36	7	37	-39	3	33	31			

connects equivalent chains in different unit cells by forming O – Na – O-bridges in the *z*-direction. The layers parallel to the *yz*-plane that are formed this way are connected by O – Na – H_2O – Na – O linkages (Fig. 2).

The $H_2Mo_5P_2O_{23}^{4-}$-group. The group differs only slightly in bond lengths and angles from the $Mo_5P_2O_{23}^{6-}$-group in (8, 5, 2).[2] It consists of five MoO_6-

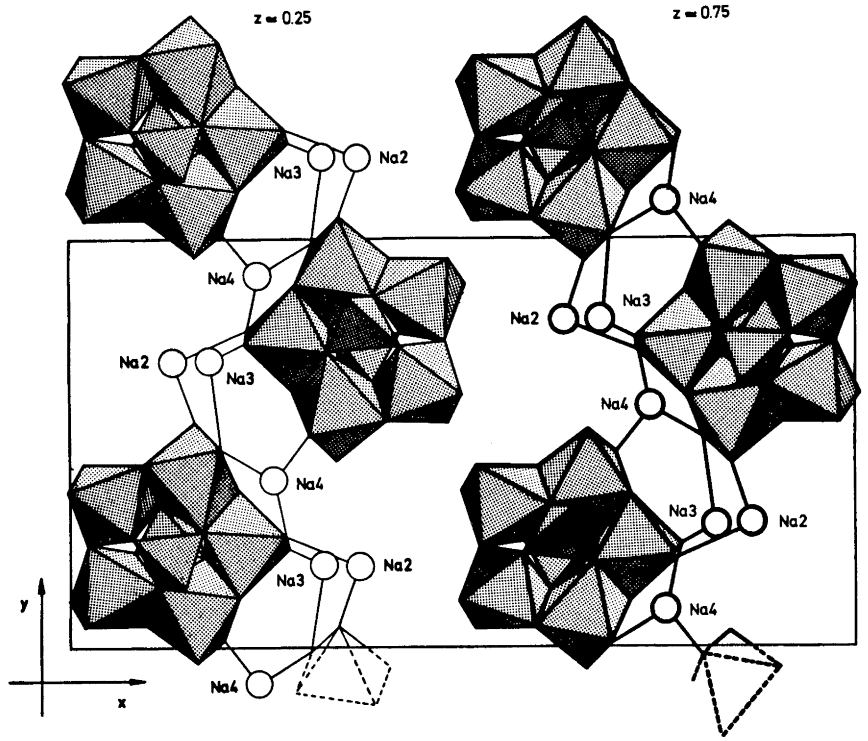

Fig. 1. A view in the $-z$-direction of the zig-zag arrangement of $H_2Mo_5P_2O_{23}^{4-}$-groups linked by three types of Na^+-bridges. The chain on $z \approx 0.75$ is drawn with thick lines.

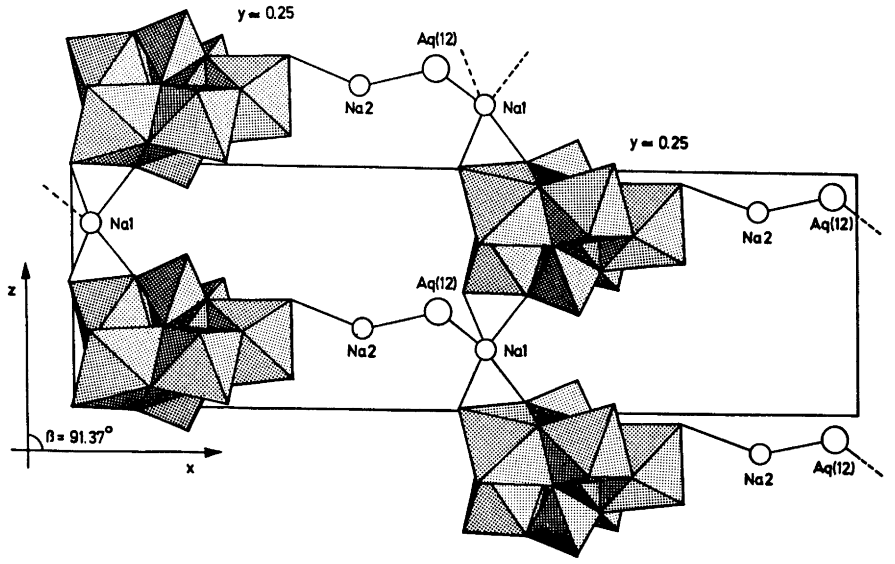

Fig. 2. A view in the y-direction of the Na^+-connections between $H_2Mo_5P_2O_{23}^{4-}$-groups in the z-direction, and the $O-Na-H_2O-Na-O$ links between layers in the x-direction.

octahedra which form a ring. The octahedra are joined together through common edges, except in one contact where they share a corner. Two PO_4-tetrahedra are attached to the ring, one above and the other below it. Each tetrahedron has three of its four oxygen atoms in common with Mo. Two of these are coordinated to two Mo atoms, the third oxygen to one Mo only. There are in all twelve unshared oxygens in the group. A stereoscopic figure of the group, including the designations of the atoms, is shown in Fig. 3. The two-fold rotation axis through Mo1 and O(34) in (8, 5, 2) is not included in this space group, but the deviations from this molecular symmetry are rather small in (10, 5, 2).

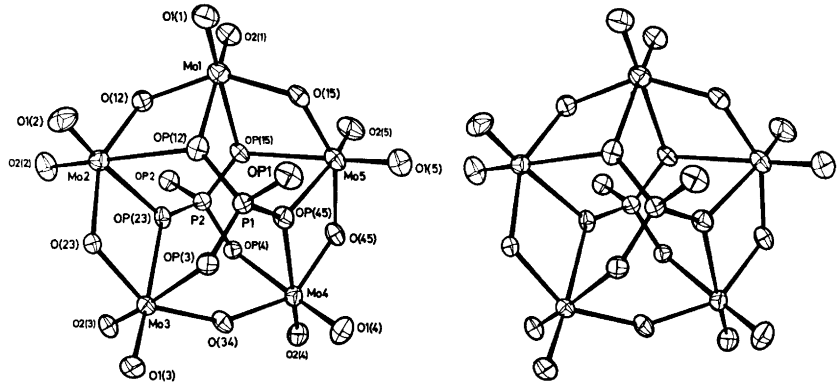

Fig. 3. Stereoscopic view of the $H_2Mo_5P_2O_{23}^{4-}$-group with thermal ellipsoids scaled to include 50 % probability.

The distances between two Mo atoms in octahedra sharing edges vary between 3.38 and 3.41 Å and increase to 3.681(1) Å when only a corner is shared (Mo3 – Mo4). The cross distances within the ring lie in the range 5.51 – 5.61 Å. The Mo – P distances vary between 3.30 and 3.61 Å while the P – P distance is 3.712(4) Å. Distances and angles between the Mo and P atoms in the group and the corresponding values for (8, 5, 2) are listed in Table 4.

A comparison shows that all the Mo – Mo distances are 0.02 – 0.06 Å longer in (10, 5, 2) than in (8, 5, 2). The P – P distance is 0.11 Å shorter in (10, 5, 2) and the P atoms seem to be pressed together. No tendency towards ring-fracture can be noted. The Mo – Mo distances between MoO_6-octahedra sharing edges can also be compared with 3.309 – 3.351 Å reported for $Na_3(CrMo_6O_{24}H_6).8\ H_2O$ [12] and 3.20 – 3.44 Å for $(NH_4)_6Mo_7O_{24}.4H_2O$.[13]

The coordination of Na^+-ions around the $H_2Mo_5P_2O_{23}^{4-}$-groups. In the structure there are four kinds of crystallographically different Na^+-ions and they are all coordinated to two $H_2Mo_5P_2O_{23}^{4-}$-groups at the same time. Na1, which is the atom that connects groups in the z-direction, coordinates O1(3) and OP(3) from one group and O2(4) and OP(4) from the other. Na2 and Na3 are both attached to two oxygen atoms, one in each group. For Na2 the oxygen

Table 4. Distances (Å) and angles (degrees) within the $H_2Mo_5P_2O_{23}^{4-}$-group (and for the Mo and P atoms in the $Mo_5P_2O_{23}^{6-}$-group in (8,5,2)).
The designation of the atoms is explained in Table 1. The estimated standard deviations are given in parentheses and refer to the last decimal place given. The values are based on parameters from block-diagonal least squares refinements.

	(10,5,2)	(8,5,2)		(10,5,2)	(8,5,2)
Mo1–Mo2	3.375(1)	3.364(1)	P1-Mo1	3.461(3)	3.439(3)
Mo1–Mo3	5.507(1)	5.459(2)	P1-Mo2	3.521(3)	3.505(3)
Mo1–Mo4	5.520(1)	5.459(2)	P1-Mo3	3.303(3)	3.335(3)
Mo1–Mo5	3.405(1)	3.364(1)	P1-Mo4	3.602(3)	3.644(3)
Mo2–Mo3	3.389(1)	3.356(1)	P1-Mo5	3.401(3)	3.432(3)
Mo2–Mo4	5.608(1)	5.566(1)	P2-Mo1	3.482(3)	3.439(3)
Mo2–Mo5	5.526(1)	5.493(2)	P2-Mo2	3.409(3)	3.432(3)
Mo3–Mo4	3.681(1)	3.647(2)	P2-Mo3	3.606(3)	3.644(3)
Mo3–Mo5	5.609(1)	5.566(1)	P2-Mo4	3.306(3)	3.335(3)
Mo4–Mo5	3.391(1)	3.356(1)	P2-Mo5	3.534(3)	3.505(3)
			P1-P2	3.712(4)	3.822(6)
	(10,5,2)	(8,5,2)			
Mo2–Mo1–Mo5	109.19(3)	109.44(5)			
Mo3–Mo2–Mo1	109.00(3)	108.63(4)			
Mo4–Mo3–Mo2	104.89(3)	105.18(3)			
Mo5–Mo4–Mo3	104.89(3)	105.18(3)			
Mo1–Mo5–Mo4	108.63(3)	108.63(4)			

	O1(1)	O2(1)	O(12)	O(15)	OP(12)	OP(15)
Mo1	1.713(9)	1.701(8)	1.919(7)	1.928(7)	2.313(7)	2.361(7)
O1(1)		2.665(13)	2.830(11)	2.801(11)	2.828(10)	
OP(15)		2.869(10)	2.773(10)	2.562(11)	3.052(11)	
O(12)		2.767(11)			2.549(10)	
O(15)		2.812(11)			2.766(10)	
O1(1)–Mo1–		102.7(4)	102.3(4)	100.4(4)	87.9(4)	
OP(15)–Mo1–		88.3(4)	80.0(3)	72.6(3)	81.5(3)	
O(12)–Mo1–		99.5(4)			73.4(3)	
O(15)–Mo1–		101.4(4)			80.9(3)	

	O1(2)	O2(2)	O(12)	O(23)	OP(12)	OP(23)
Mo2	1.703(8)	1.697(8)	1.921(7)	1.951(7)	2.388(7)	2.212(7)
O1(2)		2.701(12)	2.837(12)	2.718(10)	2.882(11)	
OP(23)		2.941(10)	2.741(9)	2.453(11)	2.705(10)	
O(12)		2.704(10)			2.549(10)	
O(23)		2.774(11)			3.037(10)	
O1(2)–Mo2–		105.2(4)	102.9(4)	95.9(3)	87.9(4)	
OP(23)–Mo2–		96.7(4)	82.8(3)	71.9(3)	71.9(3)	
O(12)–Mo2–		96.6(4)			71.6(3)	
O(23)–Mo2–		98.8(4)			88.3(3)	

	O1(3)	O2(3)	O(23)	O(34)	OP(3)	OP(23)
Mo3	1.702(8)	1.735(8)	1.911(7)	1.898(7)	2.275(7)	2.354(7)
O1(3)		2.687(11)	2.790(10)	2.806(11)	2.696(10)	
OP(23)		2.868(10)	2.453(11)	2.845(10)	3.143(11)	
O(23)		2.811(11)			2.650(10)	
O(34)		2.752(10)			2.684(11)	

Table 4. Continued.

O1(3)–Mo3–		102.8(4)	100.9(4)	102.3(3)	84.1(3)	
OP(23)–Mo3–		87.7(3)	69.3(3)	83.3(3)	85.5(3)	
O(23)–Mo3–		100.8(3)			78.1(3)	
O(34)–Mo3–		98.4(3)			79.5(3)	
	O1(4)	O2(4)	O(34)	O(45)	OP(4)	OP(45)
Mo4	1.715(9)	1.702(9)	1.915(7)	1.898(7)	2.273(7)	2.343(7)
O1(4)		2.674(13)	2.745(11)	2.787(11)		2.863(11)
OP(4)		2.682(10)	2.676(11)	2.670(10)		3.130(11)
O(34)		2.811(12)				2.850(10)
O(45)		2.784(11)				2.434(11)
O1(4)–Mo4–		103.0(4)	98.1(4)	100.8(4)		88.3(4)
OP(4)–Mo4–		83.6(3)	78.9(3)	79.0(3)		85.4(3)
O(34)–Mo4–		101.9(4)				83.4(3)
O(45)–Mo4–		101.2(4)				69.2(3)
	O1(5)	O2(5)	O(15)	O(45)	OP(15)	OP(45)
Mo5	1.701(9)	1.709(10)	1.914(7)	1.968(7)	2.414(7)	2.195(7)
O1(5)		2.710(14)	2.718(11)	2.781(12)		2.916(11)
OP(15)		2.920(12)	2.562(11)	3.057(10)		2.720(11)
O(15)		2.850(12)				2.739(10)
O(45)		2.721(11)				2.434(11)
O1(5)–Mo5–		105.2(5)	97.3(4)	98.3(4)		96.1(4)
OP(15)–Mo5–		88.5(4)	71.5(3)	87.9(3)		72.2(3)
O(15)–Mo5–		103.6(4)				83.3(3)
O(45)–Mo5–		95.2(4)				71.3(3)
	OP1	OP(3)	OP(12)	OP(45)		
P1	1.564(8)	1.506(7)	1.538(7)	1.559(8)		
OP1		2.546(10)	2.458(11)	2.527(11)		
OP(3)			2.525(10)	2.493(11)		
OP(12)				2.550(10)		
OP1–P1–		112.1(4)	104.8(4)	108.1(4)		
OP(3)–P1–			112.1(4)	108.9(4)		
OP(12)–P1–				110.8(4)		
	OP2	OP(4)	OP(15)	OP(23)		
P2	1.565(8)	1.504(7)	1.530(7)	1.545(8)		
OP2		2.537(10)	2.456(11)	2.518(11)		
OP(4)			2.527(9)	2.463(10)		
OP(15)				2.546(10)		
OP2–P2–		111.5(4)	105.0(4)	108.1(4)		
OP(4)–P2–			112.8(4)	107.7(4)		
OP(15)–P2–				111.7(5)		

atoms are O1(1) and O2(2) and for Na3 O2(1) and O1(2) in group one and two, respectively. Na4 is in contact with O1(1) and O1(2) in one group and with O2(5) in another. (Na2–4 are the bridge ions in the previously mentioned zig-zag chains.) Consequently there are eight sodium ions coordinated to seven of the twelve unshared oxygen atoms and to two of the shared oxygen atoms in a $H_2Mo_5P_2O_{23}^{4-}$-group. Since every ion is shared between two groups the average number of Na^+-ions around a group is four, which implies that the

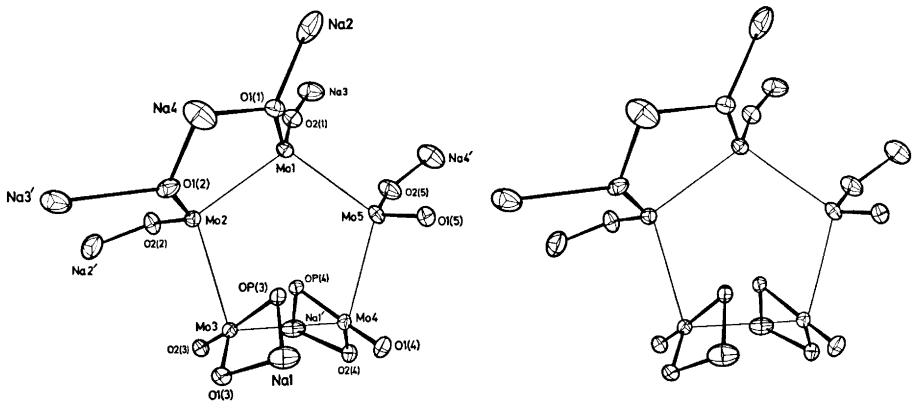

Fig. 4. Stereoscopic view of the sodium coordination to the $H_2Mo_5P_2O_{23}^{4-}$-group (for clarity all shared oxygen atoms except two have been omitted). The thermal ellipsoids are scaled to include 50 % probability.

charge of the group has been neutralized. The configuration of Na^+-ions around a group is shown in Fig. 4.

The sodium-oxygen arrangement. Every sodium ion is surrounded by six group- or water-oxygen atoms forming an octahedron, which can be written schematically as $NaO_x(H_2O)_{6-x}$. For Na1 $x=4$, for Na2 and Na3 $x=2$, and for Na4 $x=3$. The octahedra are coupled together to form an $Na_4O_9(H_2O)_8$-unit by sharing oxygen atoms as shown in Fig. 5.

The Na1 octahedron has a corner [Aq(12)] in common with the Na2 octahedron, while the latter also shares Aq2(23) with the Na3 octahedron and O1(1) with the Na4 octahedron. The Na3 and Na4 octahedra share an edge through Aq1(34) and Aq2(34). The $Na_4O_9(H_2O)_8$-unit is the smallest unit

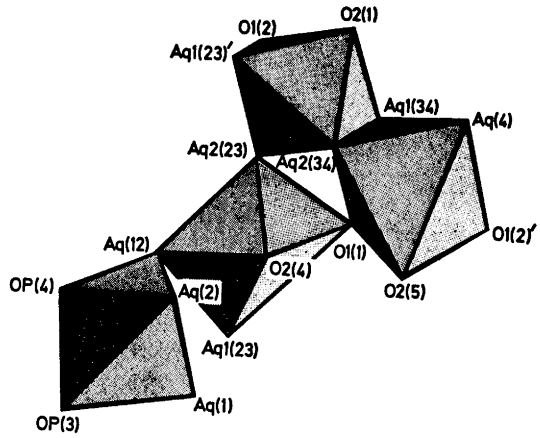

Fig. 5. The $Na_4O_9(H_2O)_8$-unit schematically drawn with octahedra.

necessary to describe the network that is formed since Aq1(23) and O1(2) are also shared with other units. The Na – Na distances are in the range 3.61 – 4.83 Å.

The two "free" water molecules. There are two water molecules, Aq1 and Aq2, which are not coordinated to any Na^+-ion. They are situated one on each side of the $H_2Mo_5P_2O_{23}^{4-}$-group, Aq1 2.617(12) Å from OP1 and Aq2 2.613(12) Å from OP2. They also seem to be related by the near two-fold rotation axis mentioned.

The MoO_6-octahedra. The MoO_6-octahedra are somewhat distorted from an ideal octahedron and the Mo – O distances can be divided into three groups according to the number of atoms that the oxygen atom is coordinated to:
(1) coordinated to one Mo atom, the distance varies between 1.70 and 1.74 Å
(2) coordinated to two Mo atoms, the distance varies between 1.90 and 1.97 Å
(3) coordinated to P and to one or two Mo atoms, the distance varies between 2.20 and 2.41 Å.

This increasing distance with increasing coordination is found in (8, 5, 2) as well as in other structures referred to in an earlier paper.[2]

It is apparent that the O – O distance is shorter (2.43 – 2.56 Å) when the oxygen atoms form a shared edge between two octahedra than the distance in unshared edges (2.65 – 3.14 Å). Distances and angles in the MoO_6-octahedra are listed in Table 4.

The PO_4-tetrahedra. It can be seen from the distances and angles in Table 4 that the PO_4-tetrahedra are not far from regular. The P – O distances are in the range 1.50 – 1.57 Å and the different O – P – O angles vary between 105 and 112°. These values and the values of the O – O distances (2.46 – 2.55 Å) agree well with distances found in other compounds containing phosphate groups.[14,15]

In (8, 5, 2) the shortest P – O distance (1.495(9) Å) is to the unshared oxygen, while in (10, 5, 2) this distance is the longest one [1.564(8) and 1.565(8) Å]. In the crystal structure of H_3PO_4 a significantly longer P – O distance is found when a hydrogen atom is bonded to an oxygen atom and also takes part in a hydrogen bond than when no hydrogen atom is present.[14] The difference found between (8, 5, 2) and (10, 5, 2) can probably be explained in the same way. The hydrogen atoms in the $H_2Mo_5P_2O_{23}^{4-}$-group could, if situated on one unshared P-oxygen each, cause the elongation in the P – O distance especially if a suitable hydrogen bond to some other atom occurred. The two non-coordinated water molecules are situated at reasonable hydrogen bond distances from these oxygen atoms. However, no definite positions of the hydrogen atoms are available to prove this assumption.

The sodium-oxygen octahedra. The octahedra are quite distorted from an ideal octahedron with Na – O distances in the range 2.21 – 2.63 Å, with five exceptions (Table 5). Three of these occur when the same group oxygen is shared between different sodium ions [2.694(10), 2.753(11) and 3.038(11) Å]. The other two [2.733(10) and 2.811(10) Å] are in the octahedron around Na1, which is the most distorted one since four of its oxygens are $H_2Mo_5P_2O_{23}^{4-}$-oxygens and dominated by the coordination to Mo-atoms.

Table 5. Distances (Å) within the sodium – oxygen octahedra. The designation of the atoms is explained in Table 1. The estimated standard deviations are given in parentheses and refer to the last decimal place given. The values are based on parameters from block-diagonal least squares refinements.

	O1(3)	O2(4)	OP(3)	OP(4)	Aq(1)	Aq(12)
Na1	2.811(10)	2.733(10)	2.341(9)	2.343(9)	2.374(11)	2.431(11)
O1(3)			2.696(10)	4.858(11)	3.353(12)	3.415(13)
O2(4)			4.763(12)	2.683(10)	3.353(14)	3.385(13)
OP(3)				3.665(11)	3.297(12)	
Aq(12)				3.477(12)	3.782(14)	
	O1(1)	O2(2)	Aq(2)	Aq(12)	Aq1(23)	Aq2(23)
Na2	2.694(10)	2.274(10)	2.208(15)	2.633(12)	2.604(14)	2.482(13)
O1(1)		3.783(11)	3.244(15)		4.581(14)	3.167(13)
Aq(12)		3.623(13)	3.225(16)		3.301(15)	3.682(14)
O2(2)					3.000(13)	3.122(14)
Aq(2)					3.888(21)	3.446(16)
	O2(1)	O1(2)	Aq1(23)	Aq2(23)	Aq1(34)	Aq2(34)
Na3	2.331(10)	3.038(11)	2.423(12)	2.331(12)	2.374(11)	2.452(14)
O2(1)		3.787(12)	3.194(12)		2.881(14)	3.310(16)
Aq2(23)		3.401(13)	3.789(15)		3.491(15)	3.856(16)
O1(2)			3.800(13)		4.161(15)	
Aq2(34)			3.342(17)		3.253(16)	
	O1(1)	O1(2)	O2(5)	Aq(4)	Aq1(34)	Aq2(34)
Na4	2.753(11)	2.442(10)	2.528(12)	2.417(12)	2.517(15)	2.421(14)
O1(1)		3.744(11)	3.460(13)		2.942(14)	3.805(17)
Aq(4)		3.510(13)	4.059(14)		3.785(16)	3.238(15)
O1(2)			3.039(11)		4.139(15)	
Aq2(34)			3.549(18)		3.253(16)	

There is no significant difference between the Na – O distances arising from water oxygen atoms or group oxygen atoms and no systematic effects on the distortion of the octahedra apart from those mentioned are evident.

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