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Multicomponent Polyanions

VII. The Molecular and Crystal Structure of $Na_6Mo_7O_{24}(H_2O)_{14}$, a Compound Containing Sodium-coordinated Heptamolybdate Anions

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The crystal structure of $Na_6Mo_7O_{24}(H_2O)_{14}$ has been determined from three-dimensional X-ray diffraction data collected with a Philips PAILRED diffractometer, using Mo$K\alpha$-radiation. $Na_6Mo_7O_{24}$-$(H_2O)_{14}$ crystallizes in the orthorhombic space group $P2_1ab$ with unit cell dimensions $a = 15.626(1)$ Å, $b = 21.130(1)$ Å, and $c = 10.377(1)$ Å. There are four formula units in the cell. The structure has been refined by full-matrix least squares methods, with isotropic temperature factors using 2372 independent reflexions, and the final R-value is 0.056.

The structure consists of $Mo_7O_{24}^{6-}$-anions embedded in a sodium-water oxygen double-chain arrangement along the y-axis, with the sodium ions directly coordinated to the anions. The configuration of the $Mo_7O_{24}^{6-}$-anion is the same as in $(NH_4)_6Mo_7O_{24}.4H_2O$ [1-3] and $K_6Mo_7O_{24}.4H_2O$,[4] *i.e.* seven MoO_6-octahedra are joined together by common edges. Each sodium ion is octahedrally surrounded by six water and group oxygen atoms. These octahedra form chains by sharing edges and corners.

The short Mo – Mo distances are in the range 3.19 – 3.45 Å, and the Mo – O distances fall in three ranges, 1.67 – 1.76 Å, 1.88 – 2.01 Å, and 2.11 – 2.33 Å, depending on coordination number.

The first determination of a heptamolybdate structure was made by Lindqvist [1] in 1950. He investigated the paramolybdate salt $(NH_4)_6Mo_7O_{24}.4H_2O$, and concluded from a determination of the molybdenum atom positions that the compound was built up of isolated $Mo_7O_{24}^{6-}$-groups, consisting of shared MoO_6-octahedra as shown in Fig. 1. Through recent complete structure determinations of this compound, Lindqvist's structure proposal has been fully confirmed (Shimao,[2] Evans [3]). The corresponding potassium compound, $K_6Mo_7O_{24}.4H_2O$, investigated by Gatehouse,[4] has also been found to contain isolated heptamolybdate ions. An interesting question in connection with these structures is whether the cations are coordinated to the polyanions or not. From the data hitherto published no answer to the question can be given

since in the short communications presented by Evans and Gatehouse no cation positions have been listed.

In recent polyanion structure determinations it has been found that the cations are often directly coordinated to the polyanion group, thus forming a sort of cation-coordinated polyanion complex. This seems to be the case particularly when small cations like Na^+ or Li^+ are used. In the structures of $Na_6Mo_5P_2O_{23}(H_2O)_{13}$ [5] and $Na_4H_2Mo_5P_2O_{23}(H_2O)_{10}$ [6] it has been found that all Na^+-ions are directly bonded to the polyanions present in the structure ($Mo_5P_2O_{23}^{6-}$ and $H_2Mo_5P_2O_{23}^{4-}$, respectively). In order to see whether heptamolybdate anions may be directly coordinated by Na^+-ions in a similar way, we have undertaken some crystal structure investigations particularly of sodium salts crystallized from aqueous solutions.

So far the crystalline phases $Na_6Mo_7O_{24}(H_2O)_x$ with $x \approx 21-23$ and $Na_6Mo_7O_{24}(H_2O)_{14}$ have been prepared. The space group of the former compound is $P2/c$ or Pc, and the unit cell dimensions are $a = 12.91$ Å, $b = 10.07$ Å, $c = 20.14$ Å and $\beta = 126.8°$ with $Z = 2$ and $D_m \approx 2.52$ g cm^{-3}. Data collection for this compound is in progress. In the present paper the crystal structure of $Na_6Mo_7O_{24}(H_2O)_{14}$ will be described and discussed.

An additional aim of these crystal structure determinations is to obtain accurate model data for use in the large angle X-ray scattering studies of aqueous sodium heptamolybdate solutions being performed with Doc. Georg Johansson, KTH, Stockholm.[7] Preliminary results seem to indicate that the structure of heptamolybdates in solution is very similar to that of a heptamolybdate in a crystal.

EXPERIMENTAL

Crystal preparation and analyses. In a typical preparation solutions of the composition $[MoO_4^{2-}]_{tot} = 2.04$ M and $[HClO_4]_{tot} = 2.33$ M were placed for slow evaporation at room temperature and two colourless crystalline phases were obtained within a few days. The orthorhombic crystals showed a long prismatic habit while the monoclinic crystals were short prismatic. Both of them were unstable in air, and during the X-ray exposures the crystal was sealed, together with part of the mother liquid, in a glass capillary.

The content of Mo and Na was determined by elemental analyses (Department of Analytical Chemistry, University of Umeå). (Found: Mo 45.3; Na 9.6. Calc.: Mo 46.5; Na 9.5.) The content of crystal water was found to be 17.3 % (calc 17.4 %) by thermobalance analysis.

Crystal data and space group. From rotation photographs around [100] and [001], and from the corresponding Weissenberg photographs (zero, first, and second layer lines) taken with Cu$K\alpha$-radiation, the crystals were determined to be orthorhombic.

The cell dimensions were refined with a Hägg-Guinier camera with Si as internal standard (25°C). The parameters and their corresponding standard deviations are $a = 15.626 \pm 0.001$ Å, $b = 21.130 \pm 0.001$ Å, $c = 10.377 \pm 0.001$ Å and $V = 3426.3$ Å^3.

Systematic extinctions $hk0$, $k = 2n+1$ and $h0l$, $h = 2n+1$ gave two possible space groups $P2_1ab$ and $Pmab$ of which $P2_1ab$ was shown later to be the correct one (No. 29, Ref. 8). The observed density, 2.75 g cm^{-3}, was determined by flotation in a bromoform-carbon tetrachloride solution. With $Z = 4$ the calculated density is 2.80 g cm^{-3}.

Collection and reduction of intensity data. Three-dimensional intensity data were collected with a PAILRED diffractometer (equi-inclination geometry). Mo$K\alpha$-radiation monochromated with a LiF-crystal was used ($\lambda = 0.7107$ Å, 25°C). A crystal of approximate dimensions $0.21 \times 0.15 \times 0.13$ mm was mounted and rotated along the a-axis (parallel to the 0.21 mm-edge). Intensities for $0kl - 9kl$ were measured with half-scan intervals $0.6 - 1.2°$ and at a scan-speed of 0.5° min^{-1}. In all 3399 reflexions of the type hkl were

scanned up to a limit of sin $\theta \approx 0.54$. Reflexions with a relative statistical error $\Delta I_o/I_o$ greater than 0.5 were omitted which reduced the number of unique observed reflexions to 2372. The intensities were corrected for background as described in an earlier paper,[9] and for Lorentz, polarization and absorption effects ($\mu = 26.38$ 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. In direct methods the program GAASA [10] was used. Fourier summations and calculations of distances and angles were performed with programs originally written by A. Zalkin. Modified versions of LALS, written by Gantzel, Sparks and Trueblood, and LINUS, written by Hamilton and Ibers were 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.[11] The computations were carried out with a CDC 3200/3300 computer in Umeå and an IBM 360/65 computer in Gothenburg.

Crystal data:

$Na_6Mo_7O_{24}(H_2O)_{14}$ F.W. = 1445.7
Orthorhombic $P2_1ab$
$a = 15.626(1)$ Å $Z = 4$
$b = 21.130(1)$ Å $D_x = 2.80$ g cm^{-3}
$c = 10.377(1)$ Å $D_m = 2.75$ g cm^{-3}
$V = 3426.3$ Å^3 $\mu = 26.38$ cm^{-1}

STRUCTURE DETERMINATION AND REFINEMENT

The determination of the Mo atom positions was carried out with both Patterson synthesis and direct methods. The three-dimensional Patterson synthesis showed extremely strong overlapping of symmetry and cross vectors, and attempts to solve it failed at first. Direct methods were then applied, and these gave useful information of the arrangement of adjacent Mo atoms, but no descrete anions appeared. By applying the information from the direct methods to the Patterson synthesis, seven four-fold positions could be obtained. All high peaks were explained in this way. A least squares refinement at this stage gave a conventional R-value of 0.256. With standard Fourier and least squares techniques, the group oxygen, sodium and water oxygen atoms could be located. The positions of the water oxygen atoms were also confirmed in a series of difference Fourier computations.

To save computer time the refinements of the structural parameters were performed with block-diagonal least squares methods in an intermediate stage. In the final cycles, full-matrix refinements were made and a weighting scheme $w = (a + |F_o| + c|F_o|^2 + d|F_o|^3)^{-1}$ with $a = 250$, $c = -0.11$, and $d = 0.00002$ was applied. In these refinements an isotropic secondary extinction parameter was also included, as described by Coppens and Hamilton.[12] In the final cycle the resulting R-value, $R = \sum||F_o| - |F_c||/\sum|F_o|$, was 0.056, and the last shifts were less than 10 % of the estimated standard deviations for all parameters except for five isotropic temperature factors. No refinements with anisotropic thermal parameters were made, since it would have meant only five reflexions per parameter refined and extreme computer times. The atomic scattering factors used were for Mo^{3+} those given by Cromer and Waber [13] and for Na^+, O^-, and O the values in Ref. 8. Account was taken of the real part of the dispersion correction.[14] To obtain electroneutrality f(O) was used

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

	x	*y*	*z*	*B*
Mo1	0.1281 (3)	0.47122(7)	0.9476 (1)	1.043(28)
Mo2	0.1315 (3)	0.62569(8)	0.9712 (2)	1.181(29)
Mo3	0.3199 (3)	0.48018(8)	0.6701 (2)	1.146(31)
Mo4	0.3194 (3)	0.63503(8)	0.6859 (2)	1.114(30)
Mo5	0.1500[a]	0.39637(8)	0.6803 (2)	1.214(30)
Mo6	0.1276 (3)	0.55849(7)	0.6708 (1)	0.890(28)
Mo7	0.1493 (3)	0.71738(8)	0.7256 (2)	1.202(29)
O1(1)	0.1959(15)	0.4174 (7)	0.0156(14)	1.10(25)
O2(1)	0.0365(16)	0.4722 (8)	0.0450(16)	1.64(29)
O(12)	0.1849(15)	0.5468 (7)	0.0090(14)	1.19(27)
O(15)	0.0714(16)	0.4168 (8)	0.8169(15)	1.61(28)
O(126)	0.0713(14)	0.5521 (6)	0.8304(13)	0.77(23)
O(1356)	0.2024(15)	0.4800 (7)	0.7700(13)	0.97(24)
O1(2)	0.2003(18)	0.6742 (8)	0.0499(17)	2.05(32)
O2(2)	0.0411(16)	0.6216 (8)	0.0695(16)	1.75(31)
O(27)	0.0742(15)	0.6882 (7)	0.8573(15)	1.46(28)
O(2467)	0.2009(15)	0.6286 (7)	0.7894(14)	1.19(26)
O1(3)	0.3684(15)	0.4274 (8)	0.7656(16)	1.66(30)
O2(3)	0.3884(15)	0.4870 (7)	0.5390(14)	1.19(26)
O(34)	0.3512(15)	0.5546 (8)	0.7625(16)	1.84(32)
O(35)	0.2406(14)	0.4236 (7)	0.5710(14)	0.87(24)
O(346)	0.2364(16)	0.5611 (8)	0.5890(15)	1.45(28)
O1(4)	0.3621(14)	0.6836 (7)	0.8028(15)	1.26(28)
O2(4)	0.3893(18)	0.6361 (9)	0.5604(18)	2.39(36)
O(47)	0.2410(15)	0.6953 (7)	0.6092(15)	1.51(29)
O1(5)	0.2006(17)	0.3312 (8)	0.7500(16)	1.80(31)
O2(5)	0.0797(16)	0.3650 (7)	0.5699(15)	1.59(29)
O(56)	0.0816(15)	0.4943 (7)	0.5885(14)	1.16(26)
O(67)	0.0784(16)	0.6242 (8)	0.6007(15)	1.50(29)
O1(7)	0.2003(18)	0.7746 (9)	0.8084(19)	2.82(40)
O2(7)	0.0771(16)	0.7558 (7)	0.6288(13)	1.06(24)
Na1	0.4852(12)	0.3876 (6)	0.5880(12)	3.41(25)
Na2	0.5105(10)	0.5590 (5)	0.5767(10)	2.19(18)
Na3	0.4773(10)	0.7214 (5)	0.4488 (9)	2.09(18)
Na4	0.2960 (9)	0.3569 (4)	0.1322 (9)	1.75(16)
Na5	0.2946 (9)	0.5180 (4)	0.1636 (9)	1.73(16)
Na6	0.3681(10)	0.6963 (5)	0.0429(10)	2.25(19)
Aq(12)	0.5535(17)	0.4692 (9)	0.6983(17)	2.11(33)
Aq1(13)	0.5437(19)	0.2973 (9)	0.6959(18)	2.61(38)
Aq2(13)	0.3824(18)	0.3185 (9)	0.5001(20)	2.71(39)
Aq(2)	0.5673(19)	0.6151(10)	0.7406(20)	3.12(43)
Aq(36)	0.3888(19)	0.6788 (9)	0.2768(19)	2.79(40)
Aq(4)	0.4072(16)	0.3080 (9)	0.2437(17)	2.04(34)
Aq1(45)	0.3909(17)	0.4381 (9)	0.0685(17)	2.23(34)
Aq2(45)	0.2417(19)	0.4291(10)	0.2960(21)	3.27(45)
Aq(46)	0.3435(20)	0.8066(10)	0.0747(21)	3.36(46)
Aq1(5)	0.4132(19)	0.5437(10)	0.2963(22)	3.27(46)
Aq2(5)	0.2207(16)	0.5788 (8)	0.3218(19)	2.23(34)
Aq(56)	0.3767(15)	0.5854 (7)	0.0242(14)	1.14(26)
Aq(6)	0.5219(26)	0.7097(15)	0.0384(30)	6.01(74)
Aq	0.2232(17)	0.7159 (9)	0.3529(18)	2.26(35)

[a] Arbitrarily fixed.

Table 2. Observed and calculated structure factors. The columns are k, $|F_o|$, $|F_c|$ and phase angle α (radians), respectively.

	0 K 14		
0	149	139	3.14
2	92	88	-3.14
3	48	43	-3.14
4	55	67	0.00
5	48	40	-0.00
	0 K 13		
9	58	40	3.14
4	53	60	-3.14
3	61	55	-3.14
0	60	46	3.14
	0 K 12		
0	59	67	0.0
1	58	50	-3.14
2	104	112	-0.00
6	49	40	3.14
8	69	55	-3.14
11	143	132	3.14
12	46	42	0.00
13	68	81	3.14
	0 K 11		
18	85	81	-0.00
17	73	80	3.14
16	45	63	3.14
15	65	64	3.14
14	63	71	-0.00
13	50	50	-3.14
12	43	53	0.00
11	137	133	3.14
9	98	113	3.14
8	48	63	3.14
7	40	34	0.00
5	71	69	-0.00
4	93	106	0.00
2	192	198	-3.14
1	86	83	-3.14
0	258	249	3.14
	0 K 10		
0	69	82	3.14
2	74	63	-3.14
3	116	111	-3.14
4	118	130	3.14
5	102	105	-0.00
6	54	55	-3.14
9	90	86	3.14
11	110	113	-0.00
13	179	175	-0.00
15	138	132	-0.00
16	56	55	-0.00
17	113	111	3.14
20	54	60	-0.00
	0 K 9		
20	71	64	-0.00
16	100	94	-0.00
13	61	67	3.14
12	53	50	0.00
11	107	103	3.14
10	39	45	3.14
7	109	108	-0.00
6	57	60	3.14
5	41	37	0.00
4	120	116	3.14
2	132	138	0.00
0	57	62	0.0
	0 K 8		
0	376	365	3.14
1	123	119	-3.14
2	224	227	-3.14
7	109	109	0.00
8	56	61	-3.14
11	140	146	3.14
12	77	86	-0.00
13	38	32	-0.00
14	43	30	0.00
15	76	87	3.14
18	40	55	-0.00
19	71	87	-3.14
21	46	31	-0.00
24	101	103	-0.00
	0 K 7		
22	70	80	-0.00
21	75	69	-0.00
19	39	33	3.14
18	66	54	-0.00
17	100	100	-3.14
15	162	169	-0.00
14	127	131	-0.00
13	286	287	-0.00
12	43	55	-3.14
11	227	232	-0.00
10	38	18	-0.00
9	66	57	-3.14
8	48	47	0.00
7	82	82	-0.00
6	76	63	-3.14
5	195	189	-0.00
4	111	111	3.14
3	63	75	3.14
2	107	99	-3.14
1	40	43	0.00
0	98	99	0.0
	0 K 6		
0	225	220	0.0
1	38	40	0.00
2	198	192	-0.00
3	49	52	3.14
4	88	88	3.14
5	65	56	0.00
7	134	136	-0.00
8	78	78	0.00
10	41	21	-3.14
13	70	69	3.14
15	139	137	-0.00
16	63	55	-0.00
17	38	20	3.14
19	45	38	3.14
21	40	46	3.14
24	83	84	3.14
26	109	111	3.14
	0 K 5		
26	106	108	-0.00
24	109	118	-0.00
19	89	92	3.14
17	46	43	-0.00
16	108	101	-0.00
15	77	70	3.14
12	64	60	0.00
11	154	162	3.14
7	211	207	-0.00
5	46	39	-0.00
1	35	28	0.00
0	167	175	3.14
	0 K 4		
0	193	180	0.0
1	37	19	-0.00
2	114	110	-3.14
5	99	104	-0.00
7	213	216	-0.00
9	35	40	-3.14
10	59	59	-0.00
11	230	229	-0.00
12	108	101	-3.14
13	365	371	-0.00
16	48	52	3.14
17	71	81	-3.14
19	89	96	3.14
20	116	117	3.14
21	73	65	-0.00
22	46	39	-0.00
24	99	97	0.00
25	131	134	3.14
	0 K 3		
27	52	51	3.14
26	152	149	3.14
24	59	54	3.14
22	59	59	3.14
21	76	69	3.14
20	64	66	3.14
17	49	58	3.14
15	125	127	-0.00
13	45	53	3.14
12	240	240	3.14
11	180	179	-0.00
8	104	112	-0.00
6	120	114	-3.14
5	78	82	-0.00
4	93	94	-3.14
3	158	150	3.14
2	263	253	-0.00
1	180	173	-0.00
0	749	803	0.0
	0 K 2		
0	239	216	3.14
2	72	71	-0.00
4	49	58	3.14
5	85	88	-0.00
6	92	89	-0.00
7	122	117	-0.00
8	69	79	-0.00
10	36	31	3.14
11	178	175	3.14
13	216	211	3.14
14	104	103	3.14
15	50	63	3.14
16	71	67	-0.00
17	50	60	-0.00
18	115	118	3.14
20	61	68	3.14
23	40	12	-3.14
24	108	112	-0.00
25	41	24	-0.00
26	108	116	-0.00
27	44	41	3.14
	0 K 1		
26	78	79	-0.00
25	101	94	-3.14
24	94	99	-0.00
23	82	77	-3.14
21	81	72	0.00
20	107	109	3.14
18	146	148	3.14
16	40	36	3.14
15	127	137	0.00
14	130	126	-3.14
13	554	551	-0.00
12	97	99	-3.14
11	256	254	-0.00
8	29	18	-3.14
7	90	81	-0.00
6	122	117	-0.00
5	87	77	0.00
4	30	29	-3.14
3	122	119	-0.00
	0 K 0		
4	71	68	-3.14
10	56	58	0.00
12	404	404	3.14
14	72	76	-0.00
16	67	67	-0.00
20	184	190	3.14
22	38	35	3.14
24	124	112	3.14
26	193	200	3.14
	1 K 14		
1	69	63	-0.55
3	91	85	-0.20
5	86	77	-0.36
	1 K 13		
10	47	45	-1.64
8	83	93	2.74
6	52	44	1.11
5	96	91	-1.02
1	87	93	2.96
	1 K 12		
1	81	88	-0.10
2	46	29	0.32
3	87	75	-1.07
4	87	78	2.44
6	113	110	1.99
7	42	39	0.32
8	65	64	2.20
9	42	45	1.78
11	49	52	-1.42
12	90	81	0.01
15	54	58	1.96
	1 K 11		
18	77	87	-0.76
15	54	47	2.82
14	140	139	2.86
12	134	126	2.87
10	105	113	2.46
9	93	88	2.41
8	41	27	-0.33
7	74	67	2.38
6	97	102	2.99
3	115	115	-0.34
1	59	66	-0.14
	1 K 10		
1	205	196	2.99
3	55	47	-2.21
4	50	23	2.91
5	144	145	-0.76
6	58	55	1.84
7	107	116	3.01
8	114	113	2.85
10	89	85	2.52
12	51	43	2.18
13	61	71	-0.69
14	41	34	1.98
15	51	55	2.70
17	110	99	2.29
18	47	30	-2.32
19	55	49	0.52
20	53	51	-0.27
	1 K 9		
20	72	68	0.02
19	63	71	-1.46
17	45	34	-2.84
16	41	47	0.77
15	58	57	1.24
14	113	110	0.21
12	121	119	0.41
11	59	58	-1.39
10	56	63	-0.22
8	157	162	2.13
7	42	45	1.33
6	122	108	1.38
4	145	136	2.15
3	101	102	-2.05
2	49	28	-1.10
1	82	81	0.45
	1 K 8		
1	117	113	0.70
2	104	103	1.28
3	135	129	-0.32
4	95	89	-2.67
5	82	89	1.65
6	110	105	-2.87
7	66	71	1.04
8	51	59	-0.26
9	138	134	2.32
10	126	120	2.35
11	99	101	-0.31
12	170	167	2.89
14	120	122	2.97
16	52	37	0.59
18	62	61	-0.56
19	73	73	-1.56
20	80	82	-2.31
21	71	73	-0.87
22	48	40	-1.31
23	100	109	2.64
24	65	54	0.03
	1 K 7		
23	65	64	-0.60
22	67	70	-0.83
19	80	81	0.63
18	40	40	-1.89
17	63	67	1.74
16	50	34	-3.05
14	58	52	2.49
13	134	127	-0.60
12	65	67	2.37
11	102	102	-0.33
10	175	173	2.64
9	63	63	-2.86
8	45	46	-2.85
7	215	212	-2.66
6	132	126	2.72
5	197	199	-0.87
4	38	49	-1.26
3	37	17	2.58
2	55	55	-2.74
1	280	279	2.67
	1 K 6		
1	116	106	1.94
2	89	84	3.07
3	109	104	2.65
4	130	121	2.07
5	37	38	-1.07
6	160	155	1.48
7	180	177	2.20
8	214	210	2.14
9	73	76	0.01
10	61	45	-0.01
12	148	148	-0.27
13	106	111	-0.71
14	172	162	-0.29
15	54	57	1.47
17	45	41	-1.63
18	88	91	2.31
19	136	138	-0.88
20	78	70	0.54
22	48	41	0.82
25	84	82	2.59
26	49	46	2.66
	1 K 5		
25	55	55	2.91
24	64	58	-0.29
23	86	95	2.57
22	60	57	-2.79
21	126	130	-0.74
20	51	57	-2.09
19	127	130	-1.16
17	112	122	-1.03
16	81	71	-0.85
14	58	60	-1.91
12	218	217	2.90
11	142	140	-0.59
10	75	70	1.85
9	169	168	2.13
8	41	41	3.13
7	70	69	2.07
6	279	277	-1.38
5	206	207	1.99
4	61	58	2.99
3	66	62	-1.16
2	63	60	2.44
	1 K 4		
1	279	284	2.64
2	72	68	-2.77
3	46	42	2.73
4	102	106	-0.91
5	93	87	-1.81
6	88	89	-0.58
7	215	216	-2.37
8	85	83	-1.06
9	207	197	-2.94
10	166	163	2.80
11	184	181	-0.17
12	46	47	-0.96
13	116	117	-0.74
15	55	61	-0.72
17	85	77	0.95
18	40	12	0.68
19	92	87	1.26
21	64	59	-0.42
22	74	63	-0.81
23	66	63	-0.74
24	49	47	2.64
25	153	152	-0.25
27	66	70	0.10
	1 K 3		
26	76	71	2.50
25	77	79	2.75
24	88	105	2.77
23	41	49	-0.10
22	74	81	-0.34
20	110	111	1.12
19	124	129	-0.84
18	93	94	1.98
17	48	40	-1.57
16	38	32	2.47
14	268	270	-0.23
13	104	102	-0.34
12	367	372	-0.34
11	59	60	-2.35
10	56	46	1.05
9	48	41	0.04
8	51	53	-0.06
7	124	122	2.27
6	99	104	0.98
4	167	162	0.25
3	130	130	2.76
2	221	204	3.09
1	97	84	1.96
	1 K 2		
1	343	339	0.29
2	83	77	1.56
3	46	50	1.97
4	40	33	-2.42
5	83	84	2.13
6	476	469	-1.09
7	137	136	0.96
8	40	40	0.12
9	72	68	0.06
10	56	52	-0.78
11	63	53	-2.50
12	172	171	2.76
13	63	61	-0.72
14	94	92	-1.81
15	69	75	0.18
16	108	105	-0.97
17	83	93	-1.40
18	69	75	2.12
19	145	141	-1.28
21	49	44	-0.84
22	51	53	2.90

Table 2. Continued

23	50	60	-2.98
24	54	59	0.23
25	143	136	2.95
26	88	94	2.36
27	68	66	-2.73
	1 K 1		
27	60	70	0.25
26	74	91	2.54
25	153	164	-0.31
24	51	56	1.81
22	36	13	-3.13
21	53	47	0.02
19	112	110	1.59
18	73	85	2.65
16	62	62	-0.97
15	50	50	-2.57
14	127	132	-1.61
13	48	57	-0.16
12	219	211	-2.36
11	127	123	-0.12
9	112	112	-3.11
8	71	79	-1.11
7	198	191	-1.78
6	326	320	-1.05
5	32	23	0.95
4	90	96	-1.27
3	61	63	-0.79
	1 K 0		
4	261	258	-0.22
6	83	68	0.99
8	89	93	-0.31
10	39	42	-3.06
12	389	388	-0.25
14	431	427	-0.41
18	109	109	2.03
20	122	130	1.48
22	90	91	-0.14
24	168	172	2.86
26	94	103	2.49
28	55	45	1.79
	2 K 14		
0	66	51	-0.68
4	79	75	1.86
6	57	65	1.23
	2 K 13		
12	70	79	1.56
11	47	38	-2.82
10	44	40	1.23
9	93	86	-1.81
8	62	43	-2.06
7	93	99	-1.73
5	81	81	-1.79
3	89	91	-1.69
0	95	98	-1.69
	2 K 12		
1	110	123	-1.61
2	53	40	-3.12
3	65	56	-1.86
4	60	73	-2.27
6	82	81	-1.74
7	61	64	1.57
8	89	90	-1.68
9	57	69	-1.98
11	106	108	-1.35
13	63	58	0.45
16	53	58	1.11
	2 K 11		
18	48	49	-2.56
17	42	36	-0.11
16	41	28	-0.93
15	43	36	0.26
14	107	121	1.56
11	56	60	-1.05
8	50	51	0.32
7	80	81	1.08
5	64	68	1.24
4	62	59	2.51
3	44	35	-0.23
2	132	135	-1.28
1	63	63	-0.70
0	92	84	-0.53
	2 K 10		
0	65	66	-1.86
1	42	59	1.55
2	40	34	-0.81
3	104	109	-1.58
4	45	38	-0.03
5	91	97	-2.45
6	47	49	-0.98
7	85	92	-1.92
9	58	52	-0.78
10	81	70	1.33
11	59	62	2.35
12	48	62	1.19
13	73	66	2.97
15	73	68	2.16
17	103	109	-1.38
19	72	71	-2.08
	2 K 9		
21	62	54	1.06
20	140	140	1.48
18	106	115	1.21
16	122	126	1.63
14	46	36	-0.96
13	52	44	0.81
12	70	71	1.56
11	83	80	-1.81
9	55	51	-2.53
8	131	129	-2.00
7	140	139	1.63
6	108	113	-1.66
5	121	111	1.28
4	138	143	-1.33
3	89	94	-1.53
2	89	92	3.07
1	142	143	-1.92
0	132	137	-2.26
	2 K 8		
0	71	73	-0.98
1	147	150	-1.27
2	133	137	-1.36
4	44	45	2.95
5	132	130	1.36
6	99	97	1.41
7	147	159	1.57
8	107	114	0.96
9	61	62	1.67
11	96	98	-1.01
13	92	89	1.38
14	106	106	1.68
15	49	59	0.40
16	50	52	1.08
18	78	70	-2.30
20	57	55	-1.95
21	70	79	1.36
22	43	49	1.56
23	47	30	1.62
24	52	63	2.01
	2 K 7		
21	102	96	-2.33
20	40	8	-1.91
19	108	112	-1.80
18	69	67	1.31
17	101	112	-1.35
15	61	57	2.05
14	70	68	2.12
13	129	122	2.52
11	93	90	2.32
10	102	105	1.30
8	36	39	-1.74
7	140	137	-2.04
6	50	45	-0.58
5	111	114	-2.35
4	49	49	0.35
3	52	49	-2.29
2	111	104	-1.51
1	47	59	0.94
0	42	51	1.16
	2 K 6		
0	192	198	3.01
1	96	91	-2.43
2	109	106	2.82
3	136	137	-1.29
4	170	169	-1.28
5	249	249	1.59
6	234	245	-1.66
7	254	255	1.72
8	231	232	-2.25
9	85	85	-2.76
13	91	97	0.97
14	51	49	-1.71
15	113	110	2.00
16	118	126	1.63
17	100	100	-1.54
18	135	141	1.38
20	142	141	1.38
24	49	44	-0.59
25	47	56	-1.86
	2 K 5		
26	48	49	-3.08
25	53	58	-1.39
24	82	79	1.93
22	59	46	1.30
21	79	78	1.23
20	96	93	-1.63
19	56	56	0.08
18	158	148	-1.64
17	56	57	1.96
16	109	112	1.60
15	60	56	-0.24
14	52	54	0.76
13	111	122	1.31
11	119	126	-0.55
10	99	103	-1.63
9	147	143	1.50
8	207	209	1.07
7	331	340	1.67
6	178	181	1.61
5	275	276	1.21
4	109	107	-2.41
3	93	92	2.05
2	47	51	1.03
1	144	144	-1.25
0	131	131	0.43
	2 K 4		
0	70	75	1.64
1	44	42	-1.65
3	100	95	1.24
4	40	37	0.15
5	77	81	-2.20
6	83	86	0.87
7	113	99	-1.52
8	209	199	1.53
9	97	95	1.35
10	34	34	0.64
11	116	113	2.25
12	138	139	-1.64
13	206	201	2.36
14	54	49	1.29
16	98	104	-1.81
17	88	86	-0.99
19	117	124	-1.83
20	127	127	-1.51
21	56	60	-2.37
24	69	61	2.26
25	92	88	-1.17
26	43	22	-1.87
27	77	77	-1.57
	2 K 3		
27	73	77	-1.27
26	62	60	-0.34
25	44	42	-1.95
24	41	34	-0.72
22	54	48	-2.01
21	55	51	-0.79
19	39	40	1.39
18	170	166	1.46
17	89	94	-1.69
15	142	136	1.67
14	87	86	-2.06
13	61	57	-0.42
12	107	111	-1.37
11	54	55	0.39
9	71	72	1.52
8	46	35	-1.45
7	113	110	2.05
6	177	179	-1.38
5	191	190	2.04
4	97	92	-0.79
3	34	36	-1.40
2	91	89	2.33
0	443	441	2.13
	2 K 2		
0	279	279	0.15
1	63	54	-2.03
2	226	230	1.56
3	39	40	0.06
4	77	83	-1.33
5	352	345	1.44
6	253	248	1.43
7	293	288	1.89
8	246	247	0.89
9	82	80	1.54
10	156	159	-1.49
11	69	69	-1.85
12	98	105	-2.21
13	82	72	0.39
14	114	113	-0.85
15	66	67	0.78
16	104	98	1.91
18	225	220	-1.51
19	100	95	1.34
20	153	161	-1.92
21	58	59	1.07
24	72	72	2.19
26	62	68	2.91
28	71	57	-1.47
	2 K 1		
28	46	40	-1.58
27	52	32	-1.85
25	61	54	-1.12
24	56	59	1.91
21	103	98	-2.57
20	198	199	-1.64
19	185	184	-1.83
18	154	148	-1.84
15	58	44	-1.81
14	86	86	-1.39
13	267	257	2.62
12	148	147	-1.58
11	59	53	2.67
10	76	74	-1.01
8	237	229	1.76
7	173	174	-2.17
6	236	224	1.64
5	332	339	-1.91
3	142	143	1.83
	2 K 0		
4	64	56	-0.78
6	344	344	-1.78
8	98	87	1.96
12	224	224	-1.69
14	123	125	-2.45
16	95	85	-1.01
18	229	221	1.21
20	65	77	-0.45
22	68	57	-1.61
24	59	53	0.57
26	87	87	-0.32
	3 K 13		
1	45	32	2.47
2	109	106	1.24
3	74	58	1.51
5	127	120	0.99
7	74	64	1.06
10	88	87	1.49
11	49	30	-1.16
	3 K 12		
15	94	105	-2.02
13	50	38	-1.65
11	87	93	1.06
9	54	52	-2.39
8	109	98	-2.09
6	141	144	-2.01
4	98	96	-2.23
3	106	101	0.97
	3 K 11		
2	73	80	-1.74
3	45	47	0.59
4	60	52	1.36
7	69	59	-2.19
8	68	81	1.53
9	90	85	-2.09
10	115	113	-1.84
14	45	40	-2.63
15	46	13	-2.46
18	88	87	1.23
	3 K 10		
19	69	74	-1.89
17	127	128	-2.21
15	41	38	-3.02
14	45	52	-2.70
13	79	75	1.13
12	70	58	-2.42
11	47	48	-1.06
10	53	48	2.64
9	57	52	1.10
8	62	60	-2.16
6	81	86	-2.27
5	189	190	1.09
3	54	52	0.63
2	65	75	1.30
1	60	46	-2.59
	3 K 9		
1	52	51	-2.41
3	97	92	1.34
4	178	174	-2.15
6	172	171	-2.18
7	134	136	-1.88
8	201	204	-2.05
11	112	114	0.89
12	56	53	-2.00
14	43	34	-2.50
15	94	90	-2.07
18	83	83	-1.98
19	135	126	1.26
21	43	39	0.54
22	55	44	-2.14
	3 K 8		
22	59	54	0.71
21	125	118	1.18
20	88	87	1.15
19	109	103	0.89
18	75	60	1.30
17	77	68	1.27
14	65	60	-2.72
13	44	33	0.54
12	64	61	-2.48
11	91	85	1.02
10	152	149	-2.00
9	179	175	-2.18
8	43	51	2.41
7	119	116	-2.81
6	153	149	1.10
5	136	137	-1.72
4	51	57	1.83
3	38	34	0.80
2	152	148	-1.82
1	143	137	-1.88
	3 K 7		
1	167	164	-2.76
2	83	81	3.05
3	50	56	-1.86
5	175	175	1.29
6	108	107	-2.24
7	95	90	1.06
8	52	43	1.13
9	64	58	0.72
10	94	91	-1.88
11	42	40	-1.25
12	48	43	1.66
13	135	134	1.16
14	38	21	-2.74
15	50	42	1.56
16	40	32	2.17
17	94	93	-2.26
18	48	48	1.34
19	77	76	-1.60
22	99	91	0.74
23	75	70	1.12
25	49	41	-1.23
	3 K 6		
25	49	47	-2.06
24	42	40	1.34
22	48	49	-2.91
21	48	58	0.44
20	58	58	-1.98
19	192	183	1.20
18	106	109	-1.99
15	61	69	-1.11
14	78	82	-0.01
13	101	101	0.93
12	62	53	-1.05
11	101	100	0.99
8	225	222	-1.94
7	233	225	-1.82
6	154	151	-2.29
5	48	42	1.55
4	174	169	-2.25
3	59	52	-2.08
2	70	72	2.46
1	128	120	-2.10
	3 K 5		
1	158	158	-1.42
2	129	119	-1.68
3	36	38	-2.87
4	36	36	-0.65
5	159	158	-1.85
6	334	338	1.04
7	209	210	-2.48
8	40	34	-0.40
9	156	163	-2.23
10	57	60	-1.99
11	121	122	1.03
12	48	42	-3.01
13	70	73	1.14
14	122	114	1.58
15	55	37	0.10
16	38	32	1.32
17	129	123	1.01
19	181	184	1.03
20	112	106	1.13
21	152	149	1.20
23	54	55	-2.20
	3 K 4		
27	61	55	-1.62
26	46	25	-3.01
25	46	25	0.31
22	104	97	1.06
21	68	67	0.42
20	42	22	-2.05
19	133	131	-1.83
17	46	58	-2.04
16	52	42	1.79
15	114	117	1.30
14	61	59	1.87
13	99	94	1.41
11	61	55	0.56
10	137	138	-1.90
9	72	74	-1.05
8	174	176	1.05
7	285	287	1.04
6	96	94	1.56
5	82	81	0.47
4	125	121	1.21
3	54	48	2.20
2	68	64	-2.08
1	117	118	-1.86
	3 K 3		
1	208	205	-2.25
2	108	103	2.28
3	150	138	-1.27

Table 2. Continued.

4	124	120	-2.64
5	193	189	1.94
6	327	309	-1.65
7	320	317	-2.66
8	105	98	-1.70
9	125	124	2.05
10	51	52	-1.12
11	63	64	1.00
12	59	57	1.05
13	135	140	0.68
14	59	64	0.21
15	63	60	-1.25
17	38	26	0.00
18	148	153	-2.16
19	140	147	1.01
20	156	165	-1.97
24	43	43	-2.24
25	54	42	-1.78
26	75	82	-2.37
27	48	42	1.09
28	50	37	-1.67

3 K 2

27	48	51	1.59
26	67	86	-2.45
24	47	40	-1.27
22	60	54	-0.90
21	67	73	1.43
20	92	89	0.94
19	260	262	1.10
18	51	55	-2.16
17	176	173	1.09
16	93	90	2.01
15	61	68	-0.79
14	147	147	1.14
13	47	45	-0.33
11	110	113	1.53
9	102	98	-1.23
8	210	204	-0.28
7	380	377	-1.67
6	464	466	0.57
5	200	198	-2.39
4	112	103	1.10
3	102	97	-1.59
2	187	176	-1.81
1	110	106	-2.00

3 K 1

3	84	79	2.06
4	214	204	0.69
5	112	100	0.59
6	454	458	1.10
7	256	259	0.99
8	138	135	0.49
9	84	82	-1.58
10	40	35	-1.43
11	44	42	0.27
13	89	90	2.33
14	172	178	1.04
15	101	98	1.77
16	60	56	1.68
17	69	70	-2.10
19	213	211	-1.91
20	57	56	1.18
24	40	45	-2.53
25	68	62	0.61
26	69	84	-2.47

3 K 0

28	74	69	-2.03
26	58	73	-2.37
24	101	98	-2.18
22	54	44	1.26
20	187	193	-1.85
18	117	118	-1.98
16	58	51	-1.06
14	134	140	0.43
12	276	282	0.98
10	49	50	-0.95
8	46	48	0.90
6	345	341	-1.63
4	41	39	0.92

4 K 14

0	113	114	-0.41
1	48	34	-1.81
2	74	67	-0.29
4	69	67	-2.70
6	49	48	-2.47

4 K 13

12	68	72	-2.39
10	48	26	-1.42
9	72	76	0.29
7	97	93	0.74
5	78	59	1.00
3	72	74	-0.23
2	49	60	-2.02
0	79	72	0.63

4 K 12

0	55	53	1.55
1	114	119	0.75
3	47	44	1.35
4	55	51	1.34
5	52	53	-1.40
6	75	67	0.85
7	69	64	-2.05
8	76	71	0.63
9	49	41	0.71
11	107	113	0.21
12	48	30	-2.52
14	43	28	2.32

4 K 11

17	43	53	-1.14
14	108	115	-2.21
12	60	73	2.08
11	92	89	-0.33
10	42	31	2.06
9	99	98	-0.67
8	50	49	-1.29
7	47	42	-2.34
6	68	70	-1.74
5	69	59	-3.06
4	42	52	-2.38
2	118	113	0.16
0	153	151	-0.67

4 K 10

0	95	85	0.10
1	76	76	-1.69
2	85	93	-0.48
3	81	83	-0.16
4	61	54	-0.62
5	65	58	1.94
7	92	86	1.03
9	67	65	0.51
10	40	39	-2.67
11	45	53	-3.11
12	57	50	-2.79
13	109	106	2.39
14	56	44	2.03
15	97	90	-3.09
17	113	106	0.50
18	54	49	-2.88

4 K 9

20	107	116	-2.60
18	78	71	-2.63
16	118	121	-2.91
15	48	42	-2.78
14	42	53	1.49
13	62	55	-2.12
12	49	57	-2.64
11	58	63	0.19
10	38	34	-0.52
8	41	38	0.86
7	103	108	-2.39
6	100	98	0.94
5	68	75	-2.10
4	124	122	0.47
3	65	62	1.18
2	76	85	-3.00
1	66	68	0.34
0	40	42	1.22

4 K 8

0	175	175	-0.68
1	68	69	0.63
2	133	133	-0.31
3	60	69	-2.25
5	136	130	3.11
6	109	109	-1.33
7	177	173	-2.73
9	63	69	-0.93
11	119	120	0.02
12	70	71	2.18
13	63	52	-1.83
14	107	104	-2.41
15	55	44	0.85
17	53	50	-1.70
18	81	83	1.80
19	48	48	0.05
20	67	72	1.08
21	55	52	-2.84
22	51	37	-2.46
23	44	34	-3.02
24	79	78	-2.98

4 K 7

24	50	60	-3.03
20	46	18	0.91
19	87	91	0.70
18	55	58	-2.51
17	113	114	0.56
16	51	55	0.99
15	108	116	2.75
14	60	60	2.92
13	230	234	2.69
11	143	150	2.97
10	77	76	-2.68
9	39	42	1.43
8	116	110	2.88
7	85	85	1.60
6	70	66	1.70
5	92	96	2.14
4	91	83	-0.99
3	49	46	-0.26
2	149	154	0.07
1	62	62	-1.24
0	52	62	-0.11

4 K 6

0	211	219	2.41
1	61	60	1.95
2	121	122	2.89
3	138	143	0.88
4	189	198	0.60
5	207	209	-2.50
6	191	188	0.98
7	164	165	-2.59
8	40	50	1.15
9	38	17	1.03
11	49	41	-2.72
12	36	29	-1.23
13	53	52	-1.56
14	55	74	0.92
15	135	131	-2.91
16	122	129	-2.95
17	64	62	0.98
18	127	124	-2.28
19	43	50	-0.79
20	111	103	-2.16
23	46	47	0.92
24	69	69	-0.60
25	60	53	0.11
26	97	91	-0.98

4 K 5

26	55	72	2.62
25	56	52	0.34
24	90	97	3.09
20	94	82	0.85
19	72	81	-0.97
18	164	160	0.88
17	59	61	-2.63
16	63	67	-2.46
15	53	54	-1.45
13	172	178	-1.88
12	82	80	1.98
11	84	88	-0.42
10	75	76	1.21
9	66	72	-1.96
8	139	134	-2.34
7	303	306	-2.57
6	149	147	-2.11
5	235	245	-2.62
4	89	85	0.66
3	93	88	-2.86
2	46	46	-0.77
1	161	162	0.96
0	228	220	-0.42

4 K 4

0	368	369	-2.32
1	65	65	-1.05
2	82	83	0.02
3	125	122	-1.71
4	80	79	-1.14
5	185	178	1.54
6	90	91	-1.79
7	161	163	1.86
8	55	51	-2.05
9	48	43	-2.07
10	58	62	3.05
11	191	195	2.82
12	110	113	0.13
13	315	322	3.00
14	48	53	-2.48
15	82	78	2.49
17	56	45	0.00
19	146	145	0.63
20	101	99	0.52
21	57	63	1.19
23	56	56	-0.72
24	53	50	3.14
25	124	123	-0.12
26	52	34	1.77
27	53	60	0.85

4 K 3

28	54	57	-0.94
27	59	55	0.17
26	104	104	-0.63
24	69	58	-0.39
22	41	38	-0.55
20	89	90	-1.34
18	142	144	-2.00
17	53	57	1.06
16	49	42	2.11
15	114	111	-2.58
14	53	55	1.18
12	173	172	-0.32
11	82	82	-2.88
10	60	67	-0.98
9	37	37	2.12
8	218	220	2.04
7	261	260	-3.09
6	219	214	1.04
5	216	212	-2.63
4	125	125	0.84
3	172	170	0.95
2	167	160	3.08
1	60	60	-2.33
0	403	418	3.10

4 K 2

0	105	104	-0.91
1	138	132	2.05
2	215	204	-2.15
3	83	78	1.24
4	75	73	0.68
5	163	174	-2.54
6	209	212	-2.83
7	285	281	-1.87
8	204	197	-2.88
9	61	57	-2.48
10	97	95	1.34
11	43	51	-0.49
13	135	131	-0.64
14	74	79	-0.17
15	93	93	-2.28
16	81	74	-2.18
18	217	220	0.53
19	53	33	-1.53
20	108	110	0.37
21	53	54	-0.91
23	38	26	-0.17
24	87	84	3.12
27	42	43	-0.32
28	79	73	0.66

4 K 1

28	45	41	0.84
27	47	37	1.63
26	55	59	2.51
25	78	77	-0.11
24	62	65	-2.77
23	46	49	-0.99
22	44	38	-0.23
20	138	134	0.38
19	136	138	0.76
18	112	118	0.51
16	44	43	-1.71
15	155	154	1.58
14	39	37	-0.37
13	251	251	2.90
12	130	132	0.01
11	128	128	2.04
10	81	78	1.68
9	41	34	-1.99
8	108	101	-1.34
7	144	144	1.25
6	81	74	-1.04
5	245	232	1.21
4	21	20	-0.17
3	216	207	-2.14

4 K 0

4	55	55	0.19
6	255	254	1.65
8	218	214	1.72
10	104	102	-1.71
12	204	206	-0.21
14	79	88	0.59
16	120	119	1.93
18	214	212	-1.65
20	55	60	-0.57
24	60	65	-0.64
26	109	113	-0.55
28	53	64	-1.35

5 K 14

2	68	60	1.77
3	94	95	2.17
5	89	95	2.40
6	59	50	-1.07

5 K 13

8	69	88	-0.37
5	88	88	2.72
2	70	73	-2.66
1	87	95	-0.90

5 K 12

1	86	88	2.70
2	42	42	-2.22
3	59	63	3.04
6	69	61	-0.58
8	55	42	-0.31
9	48	45	-0.31
10	67	66	2.24
12	73	69	2.40
14	53	49	2.10
15	46	39	0.21

5 K 11

18	51	57	2.87
15	54	34	-0.31
14	139	145	-0.73
12	138	136	-0.68
10	57	67	-0.49
9	65	47	-0.82
8	66	65	-2.76
7	48	47	-0.59
6	91	91	-0.76
5	65	69	2.19
3	106	104	2.40
2	51	55	1.07
1	58	56	2.36

5 K 10

1	202	200	-0.75
5	135	138	3.05
7	86	87	-0.53
8	82	76	-0.61
9	43	28	-2.39
10	64	80	-0.90
11	54	42	1.80
13	70	68	2.94
14	44	53	-0.47
15	72	69	-1.08
16	51	55	-0.80
17	62	64	-0.40
20	59	47	2.23

5 K 9

21	69	67	2.76
20	55	61	2.85
17	41	24	0.03
14	107	114	2.72
13	60	48	1.22
12	76	74	2.43
11	63	69	-2.50
10	65	74	2.65
8	148	154	0.03
7	49	45	1.17
4	96	99	-0.28
1	49	60	1.85

5 K 8

1	46	62	-2.67
3	92	93	2.28
4	56	49	0.09
5	48	54	0.95
6	73	70	-0.92
7	45	50	-0.65
8	46	46	-2.20
9	103	101	-0.37
10	126	126	-0.07
11	96	97	3.07
12	211	219	-0.85
13	49	46	1.80
14	131	137	-0.73
16	48	52	-2.82
17	42	42	-2.87
18	65	61	-2.95
19	56	56	2.36
20	46	39	-0.01
21	77	74	3.13
22	58	43	1.74
23	94	99	-0.58
24	83	72	2.11

5 K 7

23	75	62	3.01
22	87	102	2.71
21	57	44	2.14
19	104	101	2.09
18	46	30	-1.35
16	75	71	-0.60
15	45	44	-1.53
13	113	116	2.93
12	53	48	-1.72
11	112	119	2.02
10	147	153	-0.54
9	67	72	0.52
7	128	132	-0.37
6	42	40	-0.77
5	83	94	2.85
2	93	98	-0.24
1	372	379	-0.69

5 K 6

1	74	71	-1.76
2	106	104	-1.51
3	93	89	-0.23
4	41	41	0.03
6	92	99	1.92
7	136	139	-0.03
8	108	112	-0.14
9	86	89	-2.59
10	57	67	-2.71
12	147	157	2.64
13	80	78	2.85
14	193	190	2.45
15	47	53	1.95
17	39	35	0.97

Table 2. Continued.

18	66	78	-0.26	26	81	72	-0.73	4	86	87	1.98	7	59	63	-0.92	4	53	47	-2.91
19	122	115	3.00	25	174	169	2.69	2	118	116	-0.09	8	104	104	-1.85	5	63	69	-1.23
20	75	72	2.65	21	74	69	3.07	1	62	74	1.34	9	78	87	-2.34				
25	65	69	-0.37	20	46	41	-1.12	0	119	115	-0.31	11	101	106	-1.07		7 K 13		
				19	75	68	0.71					12	109	124	2.04	12	45	34	0.59
	5 K 5			15	89	80	-1.80		6 K 8			13	372	392	-0.96	10	52	52	-2.36
25	77	87	-0.93	13	56	53	2.20	0	214	215	2.33	14	71	76	-0.40	8	76	71	2.03
24	77	76	2.49	12	95	93	-0.49	1	99	107	2.12	15	112	116	-1.38	7	65	70	3.12
23	84	81	-0.15	11	171	176	2.58	2	131	135	1.58	17	41	46	1.64	5	118	110	-1.93
21	92	89	-3.12	10	71	77	-0.87	3	53	61	-1.34	18	51	40	-0.43	4	43	14	1.91
19	76	81	2.57	9	162	163	0.17	4	58	60	0.44	19	82	79	1.37	3	60	45	-2.11
17	51	49	2.49	8	124	134	2.56	5	128	133	-1.90	20	60	62	1.85	2	79	74	-2.34
15	39	49	2.13	7	121	122	2.78	6	42	38	-3.04	21	106	110	-0.22	1	63	58	2.46
14	106	105	-1.01	6	140	143	2.33	7	108	105	-1.51	23	58	59	1.43				
13	82	92	2.14	5	32	30	-0.69	8	87	95	3.06	24	87	84	-0.93		7 K 12		
12	227	234	-0.38	4	91	89	-2.97	10	43	49	-2.65	25	126	127	2.04	3	80	82	-2.25
11	115	115	-3.02	3	53	54	-2.75	11	114	113	2.29	26	48	16	-1.61	4	62	71	0.33
10	55	48	-0.95					12	58	44	-0.64	27	53	36	1.57	5	64	79	2.49
9	74	69	0.04		5 K 0			14	81	77	-0.86					6	104	100	0.68
7	38	43	-1.31	4	114	113	-3.11	15	90	83	3.04		6 K 3			7	56	68	-0.29
6	111	114	-2.52	6	93	98	2.70	18	43	42	-0.33	27	75	82	1.91	8	68	71	0.99
5	105	102	0.18	8	123	126	2.41	19	51	46	2.81	26	139	135	2.29	9	57	61	1.11
4	73	73	-0.29	10	64	66	1.77	20	41	10	-2.29	24	88	92	2.32	10	44	40	-0.64
3	56	51	2.37	12	425	431	2.60	21	62	62	-1.54	21	53	49	2.56	11	65	62	-2.06
2	94	99	0.60	14	289	290	2.47	23	48	22	-1.73	20	53	61	2.01	14	44	43	0.05
				16	43	43	0.53	24	85	89	-0.79	18	65	57	-2.27	15	82	72	0.89
	5 K 4			18	107	115	-0.73					17	62	57	2.22				
1	599	619	-0.65	20	48	27	-1.31		6 K 7			16	87	96	-1.86		7 K 11		
2	181	172	-0.36	22	93	88	-2.91	21	82	81	0.01	15	103	104	-1.38	18	66	58	-1.66
3	58	53	-1.38	24	155	153	-0.59	18	54	65	-0.73	13	93	93	-2.87	16	50	25	-0.11
4	127	123	2.53	26	75	86	-0.48	17	128	130	2.43	12	163	168	2.08	14	62	75	1.85
5	114	118	-2.43	28	46	32	0.64	16	44	41	-2.75	11	64	59	-0.50	12	72	72	1.88
6	49	51	0.99					15	149	152	-1.15	10	94	93	0.75	10	62	64	1.57
7	118	111	-1.47		6 K 14			14	76	86	-0.95	9	48	58	-1.44	9	67	56	0.70
8	100	104	3.03	0	125	126	2.18	13	246	248	-1.07	8	157	163	-0.66	8	65	65	-1.02
9	126	133	0.01	2	58	60	2.18	11	134	143	-0.91	7	140	146	-1.45	6	69	75	2.62
10	139	151	-0.46	3	50	63	2.42	10	47	50	-1.57	6	54	47	0.37	3	52	44	-1.45
11	170	176	2.42	4	58	67	-0.88	9	39	45	-2.24	5	207	198	-1.42	2	52	58	1.59
12	37	35	-0.89	5	49	30	-0.46	8	70	74	-1.29	4	133	132	2.34	1	37	5	1.32
13	115	111	2.78					7	69	73	-1.02	3	108	109	3.10				
14	53	64	-2.22		6 K 13			6	62	66	3.12	2	187	192	-0.96		7 K 10		
15	51	57	-1.70	12	50	40	-1.32	5	141	148	-0.57	1	158	156	-0.22	1	99	98	1.92
16	64	61	-1.27	11	63	63	-0.42	4	67	60	1.63	0	462	479	-0.78	5	133	138	-1.81
17	52	54	2.02	8	47	30	0.27	3	80	80	1.71					6	83	84	0.98
19	137	132	1.73	4	79	78	2.72	2	178	185	2.15		6 K 2			7	110	115	2.94
21	90	101	2.42	3	80	71	1.30	1	61	55	1.93	0	162	162	2.89	8	46	41	2.13
22	64	63	2.82	0	46	45	1.50	0	54	53	-1.14	2	19	18	-1.23	9	69	76	-2.90
25	145	138	2.42									3	63	58	-2.77	10	44	33	2.09
27	83	91	2.09		6 K 12				6 K 6			4	38	33	1.34	11	52	47	2.39
28	50	29	-0.30	0	57	49	-0.52	0	276	270	-0.91	5	208	207	-1.72	12	44	44	0.43
				1	66	68	2.46	1	78	78	-0.17	6	76	80	-1.91	13	64	69	-1.29
	5 K 3			2	73	65	-0.63	2	190	197	-0.87	7	213	209	-1.10	14	53	50	0.72
26	77	76	-0.34	4	50	28	-0.90	3	49	51	2.87	8	172	168	-2.50	17	87	91	0.69
25	52	54	-0.39	5	49	53	2.62	4	150	149	2.23	9	35	33	-1.88				
24	103	100	-0.56	8	47	44	1.02	5	113	114	-1.45	10	61	54	2.40		7 K 9		
22	62	50	2.91	9	61	63	0.28	6	61	64	-0.02	11	113	115	2.61	20	76	75	-0.43
21	66	68	1.80	11	104	108	2.13	7	144	150	-1.29	12	63	64	1.10	19	77	77	-2.38
20	54	51	1.62	15	44	26	2.56	8	144	149	-0.26	13	196	203	2.70	18	51	52	1.15
19	103	101	2.89	16	46	37	-1.90	9	98	99	-1.03	14	119	129	2.25	15	54	61	1.08
18	86	91	-0.12					10	68	72	1.14	16	57	56	-0.19	14	78	86	-0.65
15	65	73	2.69		6 K 11			13	83	87	-3.02	18	78	81	1.76	12	68	62	-0.12
14	302	308	2.35	18	55	54	-0.51	15	80	87	-1.17	20	113	114	1.39	11	68	79	-2.37
13	104	104	2.28	17	59	45	2.14	16	133	146	-1.33	21	83	77	2.92	10	62	74	-0.79
12	358	371	2.44	14	73	63	-0.76	18	72	80	-2.58	24	88	87	-0.93	9	71	61	0.66
10	44	45	1.70	11	112	114	2.08	19	48	37	1.84	26	99	106	-0.65	8	144	159	1.19
9	56	47	-3.08	10	52	48	-1.35	24	94	91	2.24	28	45	39	2.58	7	98	106	0.17
8	56	52	1.51	9	98	101	2.04	25	56	50	1.02					6	115	125	0.43
7	198	200	-0.22	8	103	95	2.57	26	108	97	2.09		6 K 1			5	46	58	2.99
6	321	317	1.58	4	92	96	-0.57					26	50	50	-0.51	4	133	141	0.74
5	34	33	1.81	2	137	143	2.19		6 K 5			25	109	100	2.38	3	41	53	-2.48
4	85	79	3.04	0	160	164	2.18	26	99	99	-0.77	24	85	83	-0.69	2	46	42	-0.38
3	142	135	-0.44					25	63	60	1.72	21	129	135	-0.20	1	71	79	0.36
2	140	141	-1.00		6 K 10			24	89	85	-1.06	20	96	107	1.67				
1	178	172	-2.02	0	76	71	1.41	22	41	21	2.23	19	41	38	1.44		7 K 8		
				2	69	82	1.97	21	44	44	-3.07	18	105	105	1.92	1	92	93	-0.03
	5 K 2			3	107	109	1.87	19	78	79	2.28	16	55	52	0.12	2	80	84	0.88
1	253	250	2.23	4	100	98	2.35	16	58	51	-0.80	15	60	66	2.93	3	96	93	-1.05
2	46	51	1.10	5	63	65	-0.11	15	49	41	2.94	13	341	353	-0.76	4	52	51	2.85
3	29	35	1.32	9	66	67	2.16	14	72	80	2.31	12	84	82	1.51	5	57	60	1.15
4	94	94	0.06	11	118	126	-0.58	13	95	100	2.32	11	172	170	-0.94	6	84	88	3.03
5	46	42	-0.66	12	42	38	-2.03	12	48	47	-0.34	10	58	53	1.91	7	108	111	0.18
6	229	234	2.93	13	143	143	-0.86	11	129	134	2.21	9	65	66	-2.13	9	107	103	1.08
7	193	191	0.70	15	98	100	-0.81	10	64	68	-2.64	8	169	173	-1.73	10	88	95	0.92
8	91	94	1.67	16	54	33	-1.08	9	69	65	-1.96	7	39	39	1.22	11	46	53	-1.59
9	39	43	2.84	17	116	112	2.33	8	127	131	-2.77	6	147	146	-1.30	12	119	123	1.93
11	74	77	-1.23	18	49	36	-1.77	7	105	111	-1.59	5	48	46	-0.06	13	53	54	-2.67
12	162	157	-0.22	20	66	49	-1.17	6	72	76	-1.74	4	23	19	0.54	14	74	73	1.87
13	53	58	2.50	21	58	46	-0.29	5	166	171	-2.13	3	92	93	-0.14	16	71	69	-0.56
14	44	23	-2.04					4	41	37	0.58					17	64	67	-2.29
15	98	103	1.55		6 K 9			3	90	90	-1.92		6 K 0			18	50	33	-1.26
18	45	48	-1.01	20	73	80	-1.31	2	52	51	1.18	4	36	39	2.48	19	96	107	-2.40
19	105	103	3.09	19	45	55	2.23	1	77	77	2.12	6	35	23	0.48	20	80	82	3.09
20	41	44	-2.00	18	77	73	-1.98	0	297	302	2.36	8	337	339	-1.02	21	72	85	-2.06
22	62	53	0.55	17	58	65	-0.11					10	103	111	0.89	22	73	79	-2.75
24	47	53	3.04	16	104	115	-1.24		6 K 4			12	272	277	2.18	23	71	73	1.89
25	146	148	-0.67	14	59	55	-3.10	0	152	144	0.75	16	125	123	2.72				
26	80	85	-0.49	13	45	45	-3.06	1	259	258	1.80	20	80	88	2.29		7 K 7		
27	63	68	-1.02	11	69	70	2.33	2	164	167	2.30	24	110	112	2.34	23	64	49	-1.35
28	58	51	-1.46	9	44	38	0.02	3	107	103	-0.21	26	163	165	2.38	22	88	97	-1.74
				8	61	67	0.88	4	52	51	-0.02					21	50	34	-2.76
	5 K 1			7	68	71	-1.03	5	148	139	-0.71		7 K 14			17	80	74	0.62
27	52	58	1.90	5	46	57	-2.07	6	68	69	2.48	3	46	44	-1.60	16	40	50	2.47

Table 2. Continued.

13	97	96	-1.83
10	120	134	1.82
9	62	62	2.87
7	94	96	3.04
6	53	65	2.59
5	109	115	-1.31
4	41	50	-1.25
3	51	40	-0.74
2	43	45	1.34
1	237	246	1.62
	7 K 6		
1	115	117	0.39
2	42	45	-0.43
3	44	35	2.30
4	159	163	0.63
5	35	24	2.94
6	135	140	0.37
7	139	147	1.01
8	130	138	1.63
9	49	55	-1.02
11	71	75	-2.58
12	109	101	-0.97
13	74	84	-2.33
14	115	117	-0.90
17	42	31	-2.40
18	86	95	1.22
19	133	132	-2.15
20	91	92	-0.19
25	56	60	1.86
26	70	50	1.97
	7 K 5		
24	49	56	-1.18
23	76	67	1.66
22	68	70	3.03
21	94	106	-2.27
20	83	79	-2.68
19	154	160	-2.44
17	111	117	-2.26
16	41	51	0.05
15	40	50	-2.65
14	104	108	2.38
13	69	63	-2.20
12	146	153	2.05
11	91	89	-2.13
10	78	82	0.75
9	146	154	0.74
8	46	39	-2.68
7	176	181	0.38
6	206	217	-2.05
5	128	133	1.51
4	108	111	2.63
3	82	92	-0.66
2	114	114	0.45
1	170	168	0.15
	7 K 4		
1	462	476	1.81
2	141	137	1.88
3	81	83	-0.32
4	84	91	-1.86
5	74	74	-2.11
6	134	145	-2.75
7	84	85	-2.30
8	85	93	-1.82
9	118	129	2.55
10	90	104	1.82
11	61	62	-1.67
12	40	39	-1.67
13	118	130	-2.32
15	59	63	2.98
17	50	54	0.38
19	50	47	0.14
20	42	52	2.45
21	55	60	-1.96
22	87	90	-2.03
25	118	112	-0.84
	7 K 3		
26	53	64	1.23
25	60	59	2.09
24	59	66	1.59
22	60	67	-0.32
20	124	125	0.17
19	132	136	-2.12
18	106	111	0.92
15	42	41	-1.22
14	189	200	-1.29
13	62	75	-1.88
12	255	264	-1.10
11	84	85	2.92
9	92	99	-1.21
8	39	49	2.08
7	115	113	0.84
6	124	127	-0.02
5	55	48	0.50
4	134	133	-0.32
3	87	88	1.97
2	72	70	0.62
1	216	215	0.11
	7 K 2		
1	162	158	-0.56
2	81	80	0.45
3	46	48	1.53
4	113	116	-3.13
5	33	27	0.93
6	366	377	-2.09
7	257	265	0.56
8	110	109	-3.00
9	134	142	-0.04
10	48	44	-0.84
11	41	39	-2.69
12	144	148	2.44
13	56	64	-2.39
14	146	155	-2.53
15	55	73	2.99
16	66	81	-0.50
17	95	99	-2.90
18	41	44	1.54
19	144	154	-2.43
20	91	92	-2.50
21	70	68	-2.44
22	68	71	2.51
25	97	102	2.04
26	76	79	1.01
	7 K 1		
26	70	70	0.84
25	112	109	-0.95
21	52	58	-1.32
20	61	70	2.71
19	132	128	1.00
17	58	67	-0.03
16	50	53	-0.30
15	73	73	-1.49
14	39	51	-2.19
12	64	68	-2.98
11	85	91	-1.56
10	33	35	1.74
9	200	211	2.18
8	176	174	-2.29
7	223	227	-2.22
6	219	230	-2.17
5	42	36	-2.31
4	168	168	-3.14
3	96	99	-0.62
	7 K 0		
4	101	106	-0.24
6	55	52	-0.60
8	69	74	-1.81
10	81	84	2.31
12	239	241	-1.13
14	67	67	-1.37
16	58	61	2.32
18	118	126	1.25
20	146	145	0.67
22	133	123	-0.66
24	74	84	1.66
26	74	87	1.21
	8 K 13		
9	67	73	-2.80
7	103	97	-2.70
5	83	85	-3.05
3	58	59	3.05
2	45	35	1.51
0	108	101	-2.91
	8 K 12		
0	68	62	-2.76
1	110	114	-2.23
2	48	39	-2.59
3	50	48	-2.84
4	48	51	-2.58
5	74	67	0.07
6	91	92	-2.80
7	56	65	1.02
8	96	87	-2.99
9	78	85	-3.12
11	95	92	-2.35
12	48	30	0.49
13	72	62	0.79
14	57	40	-0.72
	8 K 11		
14	97	100	0.88
8	94	84	-0.03
6	83	93	0.47
4	57	56	1.72
2	78	76	-2.79
0	41	36	2.82
	8 K 10		
0	98	100	-3.02
1	47	52	1.47
3	81	74	-2.76
5	89	93	3.14
7	108	107	-2.49
9	108	103	-2.44
10	65	52	0.38
12	78	77	0.14
13	42	25	-1.41
15	62	59	0.33
17	106	102	-1.92
18	60	57	0.59
19	69	80	-3.02
	8 K 9		
20	125	128	0.74
18	129	129	0.10
16	100	111	0.51
14	79	81	-1.16
13	74	73	0.35
12	79	72	0.77
11	71	73	-2.23
10	50	41	3.04
9	85	81	-2.98
8	98	96	-3.04
7	112	111	0.43
6	134	133	-2.89
5	147	139	0.35
4	124	125	-2.20
3	54	46	-2.45
1	93	92	-2.08
0	103	107	-2.39
	8 K 8		
0	45	37	-2.80
1	71	69	-2.03
2	97	94	-2.40
3	48	51	0.29
4	56	58	2.69
5	120	120	0.29
6	94	88	0.67
7	147	151	0.54
8	116	109	-0.03
10	41	42	-0.86
13	96	88	0.55
14	117	112	0.90
17	43	49	1.36
18	53	64	-2.49
20	76	63	-2.19
21	52	58	0.31
	8 K 7		
21	78	69	2.83
19	101	112	-2.94
18	44	49	0.63
17	78	84	-2.20
16	45	52	-1.51
15	62	67	0.26
14	42	47	0.92
11	58	66	1.12
10	68	57	0.48
8	45	48	-0.02
7	60	55	-1.76
6	42	42	3.12
5	51	48	-2.70
4	45	62	1.80
3	78	78	2.82
2	77	88	-2.29
1	61	68	1.43
0	79	97	1.95
	8 K 6		
0	119	112	2.94
1	58	54	2.49
2	84	87	2.34
3	105	108	-1.95
4	141	142	-2.41
5	200	208	0.26
6	94	90	-2.80
7	115	113	0.04
8	51	67	2.65
12	41	35	1.10
13	101	97	-0.69
14	76	86	-1.84
15	93	93	0.72
16	102	98	0.30
17	71	66	-2.67
18	143	138	0.29
20	91	94	0.75
23	61	47	-2.95
	8 K 5		
25	72	74	-3.09
20	74	77	-2.65
18	146	145	-2.51
17	53	47	1.00
16	71	66	0.94
15	82	84	0.04
13	140	141	0.19
12	69	74	2.80
11	89	84	-0.86
10	75	79	-1.56
8	133	134	0.06
7	207	209	0.29
6	136	134	0.66
5	251	249	0.06
4	100	103	3.10
3	77	72	0.31
2	50	41	1.86
1	152	155	-1.96
0	176	184	-1.21
	8 K 4		
0	183	183	0.72
2	97	96	-1.84
3	122	124	1.72
4	72	80	1.47
5	134	139	-2.55
6	72	72	0.02
7	128	130	-1.66
8	114	116	0.08
9	41	37	-0.05
10	69	69	0.95
11	92	96	0.26
12	86	85	-2.09
13	81	80	0.57
15	67	65	-0.79
18	64	69	2.91
19	170	170	-2.71
20	94	93	-2.65
21	96	93	2.95
25	54	57	-2.56
27	57	66	-2.68
	8 K 3		
25	47	56	3.05
23	54	49	-2.57
20	53	44	0.90
18	152	147	0.74
17	59	57	-2.56
16	67	66	-0.67
15	117	117	0.62
14	62	69	-1.74
13	113	113	-0.02
12	103	103	-2.43
11	69	76	0.35
10	72	75	1.83
8	120	118	-2.97
7	122	124	0.15
6	192	195	-2.47
5	171	171	0.37
4	80	81	-2.37
3	137	138	-2.00
2	47	46	-0.75
0	169	167	0.72
	8 K 2		
0	295	305	-0.17
2	174	175	0.99
3	92	96	-0.95
4	58	64	-2.28
5	281	283	0.36
6	177	179	0.46
7	281	285	0.29
8	224	224	0.22
10	122	125	-1.53
12	127	132	2.99
15	80	88	1.07
16	93	96	1.50
17	37	12	1.47
18	192	194	-2.66
19	79	79	1.13
20	137	145	-2.78
21	89	89	-0.27
25	64	49	2.79
27	45	33	2.60
28	82	78	-2.27
	8 K 1		
24	49	50	0.54
23	50	40	2.24
21	111	109	2.81
20	144	144	-2.65
19	138	144	-2.59
18	152	161	-2.89
16	38	33	2.57
15	145	143	-1.78
14	67	72	2.44
13	79	87	1.77
12	129	132	-2.71
10	41	50	-1.19
9	47	49	0.50
8	245	250	0.45
7	214	211	-2.75
6	136	136	0.18
5	243	244	-2.82
3	152	157	1.72
	8 K 0		
4	22	22	-2.07
6	218	216	-2.86
8	238	239	3.02
10	79	78	1.50
12	134	136	-2.35
14	43	49	-2.12
16	113	110	-1.06
18	164	156	0.63
22	60	62	-2.87
28	54	49	1.39
	9 K 14		
3	51	61	-1.65
	9 K 13		
11	46	33	-1.62
10	60	57	0.45
5	91	91	0.23
3	63	42	-0.02
2	75	85	0.35
	9 K 12		
3	71	73	-0.06
4	71	70	2.88
5	50	64	-1.86
6	88	84	2.90
8	76	86	-2.77
11	96	94	0.85
12	49	30	-1.90
15	65	73	-2.78
	9 K 11		
14	75	81	2.18
12	87	78	1.88
10	79	68	3.05
9	70	55	2.77
8	88	87	0.73
7	46	47	2.89
6	59	58	1.25
4	49	42	0.34
3	82	80	-1.08
2	104	108	-2.19
	9 K 10		
1	84	89	2.03
2	69	67	0.58
5	172	175	0.26
6	75	78	-3.02
8	46	49	2.28
9	59	57	0.09
11	81	87	-1.72
12	63	64	2.50
13	48	50	0.51
14	53	59	2.78
15	75	66	1.87
17	95	90	-3.11
18	45	15	0.60
19	61	60	-2.67
	9 K 9		
19	75	79	0.18
18	64	66	-2.62
15	99	97	-2.68
14	55	49	-2.17
12	54	59	-2.33
11	103	109	0.33
8	166	167	-2.95
7	103	99	-3.08
6	125	118	2.89
5	50	56	-1.16
4	122	120	2.99
3	51	45	-0.07
2	79	81	1.53
1	63	61	2.99
	9 K 8		
1	69	62	-2.96
2	133	120	-2.66
3	50	39	-0.76
5	71	75	-2.57
6	112	113	0.92
7	95	86	2.60
8	64	64	1.63
9	130	127	2.99
10	90	90	2.72
11	74	82	0.37
12	78	78	2.14
14	62	53	2.03
15	50	26	-0.85
17	52	58	-0.36
18	46	41	0.39
19	81	81	-0.40
20	58	48	-0.05
21	106	100	0.08
22	44	44	-0.69
	9 K 7		
22	95	82	0.09
21	53	58	-1.32
19	84	87	-2.05
17	83	87	-2.88
15	70	76	0.90
13	81	79	-0.20
12	74	70	1.40
11	120	120	-1.67
10	94	94	2.54
8	74	81	1.13
7	54	55	1.66
6	83	83	-1.71
5	120	123	0.52
4	61	66	0.31
3	54	54	2.20
1	155	152	2.18
	9 K 6		
1	95	97	2.41

Table 2. Continued.

2	129	128	1.48	11	80	78	0.58	24	51	36	-2.58	3	53	56	-2.05	15	107	100	0.93
3	36	27	1.28	10	43	53	1.68	26	50	39	1.98	4	101	108	-1.59	14	104	107	0.01
4	120	126	-3.08	9	69	69	2.91	27	72	80	-1.68	5	133	131	-2.78	13	46	48	-1.09
6	89	85	-2.56	7	73	65	-2.70					6	350	360	0.20	12	58	60	-0.97
7	97	98	-2.83	6	183	183	0.45		9 K 3			7	239	236	-3.08	11	79	74	-1.22
8	107	105	-2.50	5	92	89	-2.57	27	51	51	0.53	8	75	78	0.09	10	36	27	0.12
9	63	58	1.14	4	66	70	-1.21	25	58	34	3.09	9	101	108	2.10	9	95	99	-1.79
10	41	33	0.20	3	39	41	-1.68	24	59	54	1.96	10	47	46	1.63	8	137	138	0.00
11	61	55	0.05	2	117	116	-2.53	22	46	42	1.53	11	75	74	0.37	7	278	282	0.57
12	89	85	-1.46	1	83	82	3.13	21	51	50	-1.15	12	43	42	1.02	6	323	331	-0.18
13	69	71	-0.61					20	105	100	3.13	13	54	34	-1.90	5	75	73	1.24
14	68	71	-1.51		9 K 4			19	114	115	-0.04	14	117	119	0.45	4	46	50	-0.62
15	48	49	-2.20	1	267	263	2.13	18	109	112	3.11	15	74	70	-1.90	3	83	86	1.12
16	53	46	-2.44	2	86	92	-2.84	17	67	55	-0.90	17	97	91	-0.27				
18	89	85	-2.90	3	74	72	1.63	16	73	76	-2.19	18	49	57	2.42		9 K 0		
19	124	127	0.00	4	91	96	0.19	14	154	152	-1.13	19	172	162	0.23	4	135	139	0.34
24	61	60	0.72	5	80	80	0.64	13	52	54	0.03	20	106	95	0.66	6	310	313	-2.05
26	50	42	-2.23	6	80	85	-0.90	12	118	123	-1.19	21	49	58	-0.36	8	128	130	-0.71
				7	159	159	0.77	9	79	77	0.60	22	48	37	-1.71	10	96	89	-1.94
	9 K 5			8	134	137	0.49	8	70	74	-1.68	26	79	78	2.86	12	185	184	-0.71
25	61	60	1.78	9	56	72	-1.94	7	167	172	-2.64	27	55	59	1.23	14	179	171	-1.28
23	61	52	3.00	10	68	67	3.06	6	195	196	-2.28					16	86	80	-2.27
22	60	57	-1.58	11	136	135	-1.02	5	62	64	0.52		9 K 1			18	92	92	2.93
21	101	98	-0.05	12	60	62	1.74	4	52	51	2.36	28	48	38	2.52	20	115	114	-3.03
20	97	97	0.27	13	84	86	-0.75	3	46	44	2.79	27	109	100	-2.11	22	78	68	1.41
19	124	120	-0.16	14	38	33	-0.37	2	130	126	1.60	26	53	71	2.70	24	80	87	2.54
17	71	75	-0.24	15	103	105	0.91	1	66	69	2.66	25	54	54	-0.59	26	72	73	2.83
15	62	65	-1.52	17	61	60	-3.02					23	56	52	-1.06	28	58	61	-2.52
14	61	50	1.07	18	51	62	1.65		9 K 2			19	187	175	-2.47				
13	94	94	-1.00	19	149	147	-2.26	1	56	56	3.12	18	43	47	2.33				
12	76	81	2.39	22	76	73	0.15	2	109	111	-2.33	17	62	56	-3.12				

for water oxygen atoms and $f(O^-)$ for the remainder. A difference Fourier synthesis based on the listed parameters showed no abnormalities. No attempts to locate hydrogen atoms were made.

Final atomic coordinates and isotropic thermal parameters and corresponding standard deviations are given in Table 1, and a comparison of observed and calculated structure factors is made in Table 2.

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

The structure is built up from $Mo_7O_{24}^{6-}$-ions, Na^+-ions and H_2O molecules. The $Mo_7O_{24}^{6-}$-ion consists of seven MoO_6-octahedra joined together by sharing edges as shown in Fig. 1.

A characteristic feature of the structure is that all Na^+-ions are directly coordinated to $Mo_7O_{24}^{6-}$-groups, and most of them act as links in $O-Na-O$

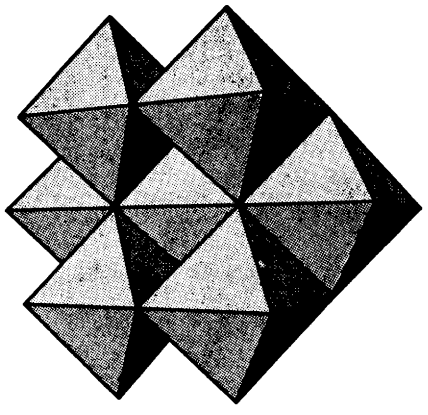

Fig. 1. The $Mo_7O_{24}^{6-}$-anion schematically drawn as a regular polyhedron.

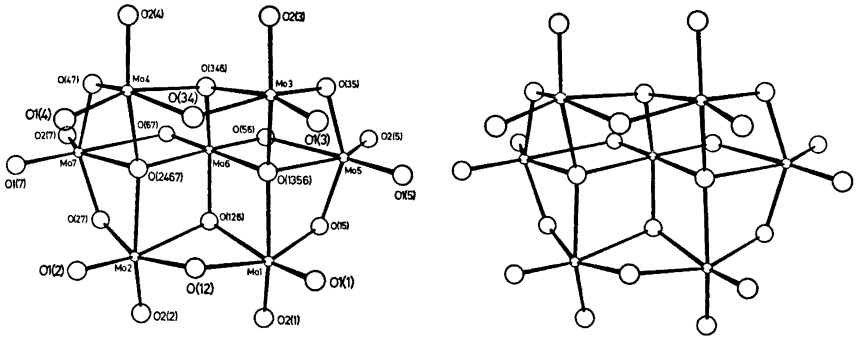

Fig. 2. A stereoscopic view of the $Mo_7O_{24}^{6-}$-anion.

bridges in the x-, y-, and z-directions. In Fig. 3 these connections are illustrated schematically.

Each Na^+-ion is octahedrally surrounded by oxygen atoms donated by both H_2O molecules and $Mo_7O_{24}^{6-}$-groups. The octahedra are all coupled together through common edges and corners forming a double-chain arrangement in which the $Mo_7O_{24}^{6-}$-groups are embedded. The double-chains are approximately parallel with the yz-plane and stretch along the y-axis. The arrangement is shown in Fig. 4.

In the structure there are also $O-Na-H_2O-Na-O$ linkages as well as numerous hydrogen bonds indicated by short $Aq-O$ and $Aq-Aq$ distances.

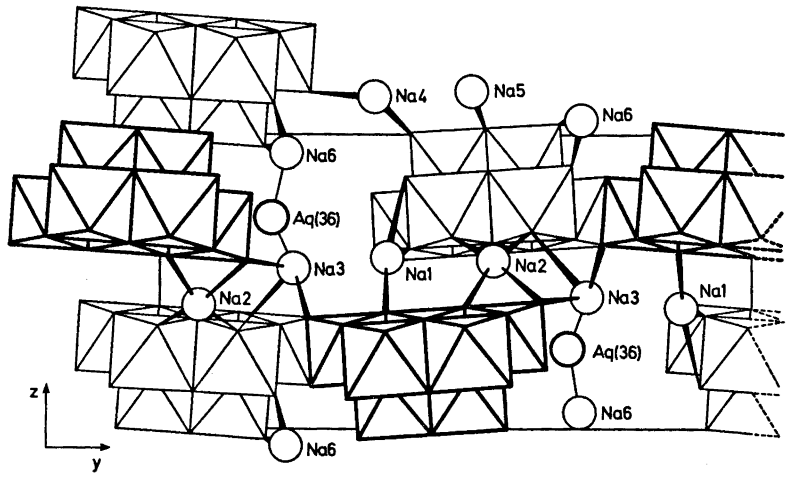

Fig. 3. A schematic drawing of all the $O-Na-O$ connections between $Mo_7O_{24}^{6-}$-anions in the structure. The $Mo_7O_{24}^{6-}$-anions are idealized and anions on $x \approx 0.7$ are drawn with thick lines, anions on $x \approx 0.2$ with thin lines.

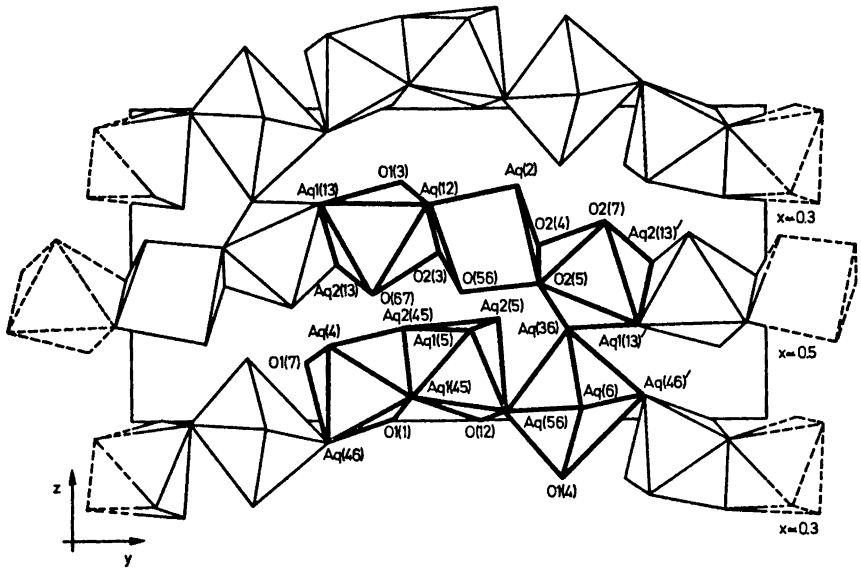

Fig. 4. A schematic drawing of the double-chain arrangement of $NaO_x(H_2O)_{6-x}$-octahedra, with repetition units in both strings marked with thick lines.

Table 3. Least squares planes through the $Mo_7O_{24}^{6-}$-group, the distances (Å) for plane-defining atoms and for some selected atoms to the planes. The selected atoms show pairs with the smallest and largest differences in distance from both planes, and an intermediate pair. The angle between the planes is 89.96°.

Plane I: $0.7062x + 0.0501y - 0.7062z - 2.9091 = 0$

Defined by				Samples			
Mo5	0.002	O(56)	0.021	O(126)	−1.805	O1(1)	−1.930
Mo6	−0.008	O(67)	0.034	O(346)	1.795	O1(3)	1.816
Mo7	−0.002	O1(5)	−0.023	O(27)	−1.824	O1(2)	−1.861
O(1356)	0.007	O1(7)	0.015	O(47)	1.840	O1(4)	1.746
O(2467)	0.007	O2(5)	−0.001	O2(2)	−3.818		
		O2(7)	−0.048	O2(4)	3.772		

Plane II: $-0.0004x - 0.9975y - 0.0701z - 12.2533 = 0$

Defined by				Samples			
Mo6	−0.007	O(12)	0.006	O(1356)	1.574	O(56)	1.406
O(126)	0.012	O(34)	0.012	O(2467)	−1.572	O(67)	−1.342
O(346)	−0.003			O(15)	2.874	O2(1)	1.540
				O(27)	−2.877	O2(2)	−1.627
				O2(3)	1.594		
				O2(4)	−1.564		

Table 4. Distances (Å) and angles (degrees) within the $Mo_7O_{24}^{6-}$-group. 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.

Mo1 – Mo2	3.274(2)	Mo1 – Mo6 – Mo2	57.20 (5)
Mo3 – Mo4	3.276(2)	Mo1 – Mo6 – Mo3	74.90 (9)
Mo1 – Mo5	3.211(2)	Mo1 – Mo6 – Mo4	102.46(11)
Mo2 – Mo7	3.214(2)	Mo1 – Mo6 – Mo5	55.84 (5)
Mo3 – Mo5	3.193(4)	Mo1 – Mo6 – Mo7	112.96 (6)
Mo4 – Mo7	3.204(6)	Mo2 – Mo6 – Mo3	100.75(11)
Mo1 – Mo3	4.161(5)	Mo2 – Mo6 – Mo4	75.29 (9)
Mo2 – Mo4	4.175(5)	Mo2 – Mo6 – Mo5	112.61 (6)
Mo6 – Mo1	3.413(2)	Mo2 – Mo6 – Mo7	55.97 (5)
Mo6 – Mo2	3.426(2)	Mo3 – Mo6 – Mo4	57.23 (9)
Mo6 – Mo3	3.431(5)	Mo3 – Mo6 – Mo5	55.35 (6)
Mo6 – Mo4	3.409(6)	Mo3 – Mo6 – Mo7	112.76(14)
Mo6 – Mo5	3.445(2)	Mo4 – Mo6 – Mo5	112.40(11)
Mo6 – Mo7	3.422(2)	Mo4 – Mo6 – Mo7	55.94(10)
		Mo5 – Mo6 – Mo7	163.91(12)

	O1(1)	O2(1)	O(12)	O(15)	O(126)	O(1356)
Mo1	1.71(2)	1.75(2)	1.94(2)	1.99(2)	2.28(2)	2.19(2)
O1(1)		2.76(3)	2.74(2)	2.84(3)		2.87(2)
O(126)		2.85(2)	2.57(3)	2.86(2)		2.63(3)
O2(1)			2.83(3)	2.70(2)		
O(1356)			2.87(2)	2.49(3)		
O1(1) – Mo1 –		106.0 (9)	97.4 (8)	100.0 (8)		94.3 (8)
O(126) – Mo1 –		88.9 (8)	74.7 (7)	84.1 (6)		72.1 (6)
O2(1) – Mo1 –			100.1 (8)	92.1 (9)		
O(1356) – Mo1 –			87.9 (7)	73.2 (8)		

	O1(2)	O2(2)	O(12)	O(27)	O(126)	O(2467)
Mo2	1.70(2)	1.75(2)	1.91(2)	1.99(2)	2.33(2)	2.18(2)
O1(2)		2.73(4)	2.74(2)	2.82(3)		2.87(2)
O(126)		2.92(2)	2.57(3)	2.89(2)		2.63(3)
O2(2)			2.82(3)	2.66(2)		
O(2467)			2.87(2)	2.45(3)		
O1(2) – Mo2 –		105.2(10)	98.8 (9)	99.8 (8)		94.9 (9)
O(126) – Mo2 –		90.4 (8)	73.9 (7)	83.6 (6)		71.1 (6)
O2(2) – Mo2 –			101.0 (8)	90.9 (9)		
O(2467) – Mo2 –			89.1 (7)	72.0 (8)		

	O1(3)	O2(3)	O(34)	O(35)	O(346)	O(1356)
Mo3	1.67(2)	1.74(2)	1.91(2)	2.01(2)	2.31(2)	2.11(2)
O1(3)		2.69(2)	2.70(2)	2.84(3)		2.82(3)
O(346)		2.89(3)	2.55(3)	2.91(2)		2.60(2)
O2(3)			2.79(2)	2.69(3)		
O(1356)			2.81(3)	2.46(2)		
O1(3) – Mo3 –		103.9(10)	97.8 (8)	100.7 (8)		95.9 (9)
O(346) – Mo3 –		90.1 (8)	73.6 (8)	84.5 (7)		71.8 (7)
O2(3) – Mo3 –			99.7 (8)	91.7 (8)		
O(1356) – Mo3 –			88.7 (8)	73.3 (7)		

Table 4. Continued.

	O1(4)	O2(4)	O(34)	O(47)	O(346)	O(2467)
Mo4	1.72(2)	1.70(2)	1.94(2)	1.94(2)	2.27(2)	2.15(2)
O1(4)		2.74(3)	2.76(2)	2.77(3)		2.78(3)
O(346)		2.88(3)	2.55(3)	2.85(2)		2.58(2)
O2(4)			2.78(3)	2.68(4)		
O(2467)			2.84(3)	2.43(2)		
O1(4) –Mo4–		106.4(10)	97.7 (8)	98.2 (8)		91.1 (8)
O(346) –Mo4–		92.1 (9)	74.0 (8)	84.8 (7)		71.6 (7)
O2(4) –Mo4–			99.3 (9)	94.8(10)		
O(2467)–Mo4–			87.7 (8)	72.6 (8)		
	O1(5)	O2(5)	O(15)	O(35)	O(56)	O(1356)
Mo5	1.75(2)	1.72(2)	1.93(2)	1.90(2)	2.52(2)	2.16(2)
O1(5)		2.75(3)	2.80(3)	2.77(2)		3.15(2)
O(56)		2.74(2)	2.89(2)	2.90(3)		2.68(3)
O2(5)			2.79(2)	2.80(3)		
O(1356)			2.49(3)	2.46(2)		
O1(5) –Mo5–		105.1 (9)	99.3 (8)	98.6 (9)		107.2 (8)
O(56) –Mo5–		78.1 (7)	79.8 (7)	80.9 (7)		69.6 (6)
O2(5) –Mo5–			99.8(10)	101.2 (8)		
O(1356)–Mo5–			75.0 (8)	74.2 (6)		
	O(56)	O(67)	O(126)	O(346)	O(1356)	O(2467)
Mo6	1.76(2)	1.75(2)	1.88(2)	1.90(2)	2.27(2)	2.24(2)
O(56)		2.75(2)	2.80(2)	2.80(3)	2.68(3)	
O(2467)		2.74(3)	2.63(3)	2.58(2)	3.15(2)	
O(67)			2.83(2)	2.81(3)		
O(1356)			2.63(3)	2.60(2)		
O(56) –Mo6–		103.4 (9)	100.5 (8)	99.8 (9)	82.4 (7)	
O(2467)–Mo6–		85.9 (8)	78.7 (7)	76.7 (8)	88.3 (6)	
O(67) –Mo6–			102.6 (8)	100.6 (9)		
O(1356)–Mo6–			77.8 (7)	76.3 (7)		
	O1(7)	O2(7)	O(27)	O(47)	O(67)	O(2467)
Mo7	1.69(2)	1.71(2)	1.90(2)	1.93(2)	2.60(2)	2.15(2)
O1(7)		2.71(3)	2.73(3)	2.74(3)		3.09(3)
O(67)		2.80(2)	2.99(2)	2.95(3)		2.74(3)
O2(7)			2.77(2)	2.87(3)		
O(2467)			2.45(3)	2.43(2)		
O1(7) –Mo7–		105.7 (9)	99.1 (9)	98.1(11)		107.0 (9)
O(67) –Mo7–		77.7 (7)	81.4 (7)	79.7 (7)		69.7 (6)
O2(7) –Mo7–			99.7(10)	103.6 (8)		
O(2467)–Mo7–			74.2 (8)	72.7 (7)		

Table 5. A comparison between corresponding distances (Å) in $Na_6Mo_7O_{24}(H_2O)_{14}$ and in other structures containing $Mo_7O_{24}^{6-}$-anions.

Defining atoms	$Na_6Mo_7O_{24}(H_2O)_{14}$	$(NH_4)_6Mo_7O_{24}.4H_2O$ [1]	$(NH_4)_6Mo_7O_{24}.4H_2O$ [2]	$(NH_4)_6Mo_7O_{24}.4H_2O$ [3] (average distances)	$K_6Mo_7O_{24}.4H_2O$ [4]
Mo1–Mo2	3.274(2)	3.27	3.179	3.257	3.240
Mo3–Mo4	3.276(2)	3.28	3.250		3.253
Mo5–Mo1, Mo3	3.19–3.21	3.21–3.31	3.08–3.30	3.206	3.16–3.26
Mo7–Mo2, Mo4					
Mo6–all Mo atoms	3.41–3.45	3.29–3.48	3.18–3.50	3.405, 3.434	3.38–3.45
Mo1–Mo3	4.161(5)	4.30	4.176	–	4.272
Mo2–Mo4	4.175(5)	4.27	4.225		4.244
Mo–O	1.67–2.33 [2.52(2), 2.60(2)]	–	1.65–2.51	1.71–2.42	1.61–2.45 (1.51, 2.62)

There is also a "free" water molecule, since one of the fourteen water molecules is not coordinated to any Na^+-ion (binds to other atoms through hydrogen bonds).

The $Mo_7O_{24}^{6-}$-group. The group is shown as a polyhedron with idealized octahedra in Fig. 1, and in more detail with the designation of the atoms included, in Fig. 2.

The molybdenum atoms Mo1 – 4 are situated at the corners of an approximate rectangle, with Mo6 lying above the centre of the rectangle, and with an Mo5 – Mo6 – Mo7 angle of 163.91(12)°. The $Mo_7O_{24}^{6-}$-group has no symmetry required by the crystal symmetry, but is very close to *2mm* (C_{2v}). In Table 3 are given the equations of two least squares planes corresponding to approximate *mm*-symmetry, the atoms defining these planes, and the distances from the planes to these atoms and to some other atoms. It can be noted that the differences between corresponding distances are less than 0.12 Å. The angle between the planes is 89.96°.

As can be seen from Table 4 the Mo – Mo distances between atoms in edgesharing octahedra can be divided into three significantly different intervals, 3.19 – 3.21 Å (Mo5 – Mo1 and Mo3, Mo7 – Mo2 and Mo4), 3.27 – 3.28 Å (Mo1 – Mo2, Mo3 – Mo4) and 3.41 – 3.45 Å (Mo6 – all other Mo atoms). When sharing corners the distances are 4.161(5) and 4.175(5) Å. In Table 5 a comparison of distances between atoms in this structure and in other heptamolybdate structures is made, and the values are in agreement with those found in $K_6Mo_7O_{24}.4H_2O$ [4] and $(NH_4)_6Mo_7O_{24}.4H_2O$ according to Evans.[3] With regard to the distances given by Shimao,[2] there seems to be some discrepancy between values given and values computed from the parameters listed, thus making a relevant comparison difficult.

The MoO_6-octahedra are somewhat distorted from an ideal octahedron with Mo – O distances in three ranges depending on coordination number: 1.67 – 1.76 Å, 1.88 – 2.01 Å, and 2.11 – 2.33 Å for oxygen atoms coordinated to one, to two, and to three or four Mo atoms, respectively. In each octahedron there are two short, two intermediate, and two long Mo – O distances. Such regularities have been found previously in the structure determinations of the ammonium [3] and potassium [4] analogues, as well as in MoO_3 [15] and $Na_6Mo_5P_2O_{23}(H_2O)_{13}$.[5] The MoO_6(6) octahedron is an exception in that the three kinds of distances fall in the ranges mentioned, but the coordination is to two, three, and four Mo-atoms, respectively. The Mo – O distances Mo5 – O(56) and Mo7 – O(67) [2.52(2) and 2.60(2) Å] fall outside the ranges mentioned, and these oxygen atoms seem to be more strongly bonded to Mo6 than to Mo5 and Mo7 [distances to Mo6 1.76(2) and 1.75(2) Å]. Distances and angles in the $Mo_7O_{24}^{6-}$-group are collected in Table 4.

The sodium arrangement around and between the $Mo_7O_{24}^{6-}$-groups. The $Mo_7O_{24}^{6-}$-group has twelve unshared oxygen atoms. Na^+-ions are coordinated to nine of these and to three of the shared ones. A stereoscopic view of this coordination is shown in Fig. 5. The total number of Na^+-ions in the figure is eleven, since of the six crystallographically different Na^+-ions in the structure, Na3 is coordinated to three groups at the same time, Na1, Na2, and Na4 to two groups, and Na5 and Na6 to one group only. In this way the Na^+-ions act as links in O – Na – O bridges, connecting $Mo_7O_{24}^{6-}$-groups in the

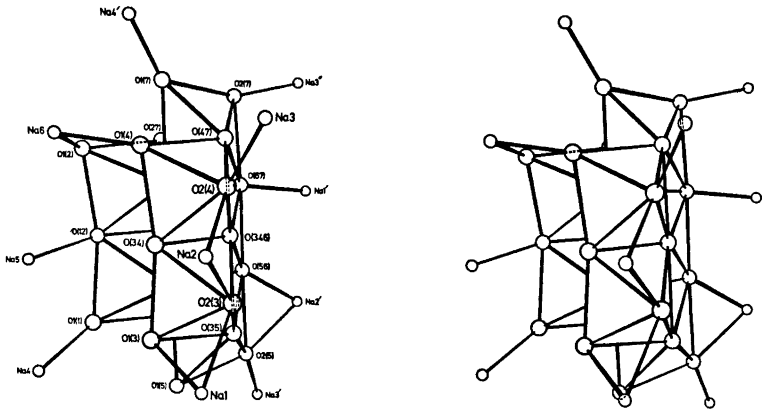

Fig. 5. A stereoscopic view of the Na^+-coordination around an $Mo_7O_{24}^{6-}$-anion. The anion is visualized as a polyhedron with spheres representing oxygen atoms.

x-, *y*-, and *z*-directions and forming a three-dimensional network. They also take part in $O-Na-H_2O-Na-O$ linkages. In Fig. 3 a schematic drawing of all the $O-Na-O$ bridges between $Mo_7O_{24}^{6-}$-groups is shown.

The sodium-oxygen arrangement. Each Na^+-ion is octahedrally surrounded by water and group oxygen atoms. The types of octahedra thus obtained may be written $NaO_x(H_2O)_{6-x}$, and there are four kinds of such arrangements in the structure, one with $x=1$, two with $x=2$, two with $x=3$, and one with $x=4$. The sodium-oxygen octahedra are all coupled together to form a double-chain arrangement by sharing edges and corners. This double-chain lies along the *y*-axis as shown in Fig. 4.

The repetition units in the two strings of the double-chain have the compositions $Na_3O_7(H_2O)_{4.5}$ and $Na_3O_5(H_2O)_{8.5}$. In Fig. 4 these repetition units are marked with thick lines. As can be seen from the figure, all three octahedra in the first unit are coupled together by sharing edges, and the connection between units is also achieved in this way. The octahedra in this unit are of the types $x=3$, 4, and 3 and with the sodium ions denoted Na1, Na2, and Na3, respectively.

In the second unit two octahedra are coupled together by sharing an edge, and the third one is connected through a shared corner. Coupling between the units is achieved by shared corners. The sodium ions in this unit are denoted Na4, Na5, and Na6, with octahedra of types $x=2$, 1, and 2, respectively.

Above and below the double-chain shown in Fig. 4 there are symmetry related chains on half a unit cell distance in *x*, and with hydrogen bonds as the only contacts. Between two different repetition units a shared water oxygen atom [Aq (36)] forms the only connection, apart from hydrogen bonds.

The sodium-oxygen octahedra are quite distorted in an irregular way, with the most distorted one, that around Na2, being close to trigonal prism. This occurs since four of its oxygen atoms are donated by two $Mo_7O_{24}^{6-}$-groups, which dominate the coordination figure. The $Na-O$ distances are in

Table 6. 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.

	O1(3)	O2(3)	O(67)	Aq(12)	Aq1(13)	Aq2(13)
Na1	2.73(3)	2.64(2)	2.45(2)	2.33(3)	2.39(3)	2.35(3)
O1(3)		2.69(2)		3.10(3)	3.95(3)	3.60(3)
O(67)		4.05(3)		3.70(2)	3.54(3)	3.46(4)
O2(3)				3.09(3)		3.58(2)
Aq1(13)				3.64(3)		3.27(4)
	O2(3)	O2(4)	O2(5)	O(56)	Aq(12)	Aq(2)
Na2	2.47(3)	2.50(3)	2.46(2)	2.33(2)	2.38(2)	2.26(3)
O2(3)		3.16(2)		3.32(3)	3.09(3)	
O2(4)			3.27(4)			3.38(4)
O2(5)				2.74(2)		3.26(3)
Aq(12)				3.11(2)		3.12(3)
	O2(4)	O2(5)	O2(7)	Aq1(13)	Aq2(13)	Aq(36)
Na3	2.55(3)	2.44(2)	2.48(2)	2.43(2)	2.59(3)	2.43(3)
O2(4)		3.27(4)	3.79(3)		3.91(3)	3.08(3)
Aq1(13)		3.71(3)	3.59(2)		3.27(4)	3.49(4)
O2(5)			3.10(2)			3.51(4)
Aq2(13)			3.68(4)			3.75(3)
	O1(1)	O1(7)	Aq(4)	Aq1(45)	Aq2(45)	Aq(46)
Na4	2.35(2)	2.38(3)	2.33(3)	2.36(2)	2.44(2)	2.51(3)
O1(1)		3.53(3)		3.13(3)	3.01(2)	3.42(3)
Aq(4)		3.35(4)		3.31(3)	3.68(3)	3.45(3)
O1(7)					3.50(3)	3.62(4)
Aq1(45)					3.32(3)	3.24(3)
	O(12)	Aq1(5)	Aq2(5)	Aq1(45)	Aq2(45)	Aq(56)
Na5	2.43(2)	2.37(3)	2.38(2)	2.47(2)	2.47(2)	2.40(2)
O(12)			3.36(3)	4.00(3)	3.98(2)	3.11(3)
Aq1(5)			3.11(4)	3.27(3)	3.61(4)	3.01(3)
Aq2(5)					3.19(3)	3.94(3)
Aq1(45)					3.32(3)	3.16(2)
	O1(2)	O1(4)	Aq(36)	Aq(46)	Aq(56)	Aq(6)
Na6	2.67(3)	2.51(2)	2.48(2)	2.39(3)	2.35(2)	2.42(4)
O1(2)		3.61(3)	3.77(4)	3.59(3)	3.35(3)	
Aq(6)		3.54(4)	3.30(4)	3.48(5)	3.47(4)	
O1(4)				3.85(3)	3.10(2)	
Aq(36)				3.49(3)	3.29(3)	

the range 2.29 – 2.71 Å and there is no significant difference in distances from Na to water oxygen or group oxygen atoms. These distances are comparable to the distances found in $Na_6Mo_5P_2O_{23}(H_2O)_{13}$ [5] and $Na_4H_2Mo_5P_2O_{23}(H_2O)_{10}$.[6] Distances within the sodium-oxygen octahedra are listed in Table 6.

The "free" water molecule. The structure also includes a water molecule which is not coordinated to any Na^+-ion, but which is probably bonded by hydrogen bonds. It is situated at about the same distance from three $Mo_7O_{24}^{6-}$-groups and has five nearest neighbour oxygen atoms at distances of 2.68 – 2.91 Å. Of these, three are water oxygen atoms [Aq1(13), Aq(36) and Aq2(5)] and two group oxygen atoms [O(47) and O1(5)]. The distances to other atoms are longer than 3.29 Å.

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