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A Refinement of the Crystal Structure of Zinc Molybdenum(IV) Oxide, $Zn_2Mo_3O_8$

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Counter intensity data for zinc molybdenum(IV) oxide, $Zn_2Mo_3O_8$, have been collected and a refinement of the structure has been carried out. The new data are consistent with space group $P6_3mc$; cell dimensions are $a=5{\cdot}759$, $c=9{\cdot}903$ Å. The refined structure confirms the presence of triangular groups of bonded molybdenum ions. The oxygen coordination scheme – octahedral (with edge sharing) around molybdenum ions, octahedral for half the zinc ions and tetrahedral for the other half – is also confirmed.

Introduction

The preparation of a number of isostructural ternary oxides of the formula type $M_2^{II}Mo_3^{IV}O_8$ was reported by McCarroll, Katz & Ward (1956, 1957). A structure determination was carried out in this earlier work using single crystals of $Mg_2Mo_3O_8$ and $Zn_2Mo_3O_8$. The main structural features of the compounds were deduced, but neither the data nor the facilities permitted an adequate refinement. For the zinc compound, the estimated probable errors were $\pm 0{\cdot}01$ Å for Mo positions, $\pm 0{\cdot}05$ Å for Zn positions, and 0·1 Å or more for O positions.

An interesting feature of these compounds is the arrangement of molybdenum ions in equilateral triangles with an inter-ion distance shorter than that in molybdenum metal. These close approaches, plus the magnetic evidence that there was no contribution to the paramagnetic moments by the *d*-orbital electrons of molybdenum (IV), led the authors to conclude that there was electron pair bonding between the molybdenum ions.

Recently, Cotton (1964) has carried out an LCAO-MO calculation for the metal atom clusters, Mo_3O_{13}, observed in these compounds. The general method of calculation has been described in a paper by Cotton & Haas (1964). His results account for the strong metal-to-metal bonding and the absence of unpaired electrons.

Because of the interesting structural features of these compounds, it had been decided some time ago to carry out a refinement of the structure when the opportunity arose. Professor Cotton's study has increased the interest in confirming the structure and improving the parameter values.

Data collection

The previously reported space group, $P6_3mc$, was consistent with the systematic absences and subsequent structure determination. Lattice constants were redetermined with a General Electric single-crystal orienter on high angle reflections with well resolved $\alpha_1\alpha_2$ peaks. Mo radiation ($\lambda K\alpha_1=0{\cdot}70926$ Å) and a 2° take-off angle were used. The lattice constants are: old, $a=5{\cdot}775\pm0{\cdot}005$, $c=9{\cdot}915\pm0{\cdot}010$ Å; new, $a=5{\cdot}759\pm0{\cdot}004$, $c=9{\cdot}903\pm0{\cdot}005$ Å.

Intensities were measured on the orienter with Mo $K\alpha$ radiation (Zr filtered), pulse height selection, and a scintillation counter by using the moving-crystal moving-counter method. Background was determined by preparing charts of background intensities at various χ settings for the 2θ range measured. The counter scan was kept large enough to include α_1 and α_2 even at the high 2θ values (100 second scans at 2° 2θ per minute).

The dimensions of the crystal used (from an original batch prepared by McCarroll) were about $0{\cdot}06\times0{\cdot}075\times0{\cdot}06$ mm. Goniostat settings for reflections up to $2\theta=110°$ were computed with a program provided by Professor David Shoemaker. The crystal was mounted with the *c* axis vertical and measurements at 3 of the 6 equivalent positions for each independent reflection were made. The intensity for each reflection was taken as the arithmetic mean of the three measurements. Intensities for all reflections with $2\theta<110°$ were measured up to $l=6$. For higher values of l the 2θ range was reduced to 75°. In all 431 intensities were measured. The reflections were divided into three groups: (*A*) those with intensities between 10 and 2400 counts above background (253 reflections); (*B*) those with counts between 5 and 10 above background (58 reflections); (*C*) those with counts less than 5 above background (120 reflections).

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Refinement

The Lorentz and polarization corrections were calculated by the Shoemaker program and were applied to the observed intensities. No absorption corrections were made. Refinement of the original McCarroll, Katz & Ward (1957) ion parameters was carried out on the IBM 7040 with the Busing–Martin–Levy least squares program. Thomas & Umeda's (1957) scattering factors, corrected for the real part of the anomalous dispersion (Dauben & Templeton, 1955), were used for Zn^{2+} and Mo^{4+}.

The refinement was begun with unit weights assigned to all reflections and isotropic temperature factors for each atom. Since the data were collected in two blocks at different times, two scale factors were used to allow for small differences.

At first temperature factors for oxygen were held fixed at zero and all other parameters were allowed to vary. Although four cycles were run, there was no significant change in positions after the first cycle. The new parameters were then used to begin four cycles with all parameters allowed to vary. Again no appreciable differences were noted after the first cycle.

Position and temperature parameters were obtained from group *A* reflections only; from groups *A* and *B* together; and from groups *A*, *B* and *C* together. The parameters obtained in all cases were well within the standard errors for group *A*. *R* indices were: group *A*, 0·038; groups $A+B$, 0·044; groups $A+B+C$, 0·072.

An anisotropic refinement of all the data was also carried out. The weighting scheme used was: $\sqrt{w}=F_o/15$ for $F_o<15$; $\sqrt{w}=1$ for $15\le F_o\le 60$; $\sqrt{w}=60/F_o$ for $F_o>60$. The final *R* index after three cycles was 0·069, and the parameter shifts for the last cycle were all considerably smaller than the standard errors. However, these standard errors were all slightly larger than those obtained by the isotropic refinement of group *A* data alone. The position parameters from the group *A* refinement were, with one exception, within one standard error of those obtained from the anisotropic refinement. (The exception was the *z* parameter for O(1), for which the group *A* refinement gave a value 0·0040 less than the value obtained from the complete

Table 1. *Atomic coordinates for atoms in* $Zn_2Mo_3O_8$*

Space group $P6_3mc$ (no. 186)

Atom	Position	x	$\sigma(x)$	z	$\sigma(z)$	T	$\sigma(T)$
Zn(1)	2(*b*)	$\frac{1}{3}$		0·9465	0·0004	0·45 Å^2	0·05
Zn(2)	2(*b*)	$\frac{1}{3}$		0·5132	0·0005	0·58	0·05
Mo	6(*c*)	0·1461	0·0001	$\frac{1}{4}$		0·16	0·01
O(1)	2(*a*)	0		0·3886	0·0026	0·43	0·30
O(2)	2(*b*)	$\frac{1}{3}$		0·1470	0·0025	0·12	0·26
O(3)	6(*c*)	0·4861	0·0015	0·3639	0·0011	0·30	0·15
O(4)	6(*c*)	0·1647	0·0016	0·6354	0·0015	0·64	0·18

Position 2(*a*): $0,0,z;\ 0,0,\frac{1}{2}+z$. Position 2(*b*): $\frac{1}{3},\frac{2}{3},z;\ \frac{2}{3},\frac{1}{3},\frac{1}{2}+z$.
Position 6(*c*): $x,\bar{x},z;\ x,2x,z;\ 2\bar{x},\bar{x},z;\ \bar{x},x,\frac{1}{2}+z;\ \bar{x},2\bar{x},\frac{1}{2}+z;\ 2x,x,\frac{1}{2}+z$.

* Group *A* reflections were used to compute parameters.

Table 2. *Bond lengths and bond angles*

			Bond lengths*		Bond angles†
A	*B*	*C*	$A-B$	$B-C$	$A-B-C$
O(1)	Mo	O(2)	2·002 ± 0·030	2·128 ± 0·030	165·4°
O(1)	Mo	O(3)	2·002 ± 0·030	2·058 ± 0·010	90·9
O(1)	Mo	O(4)	2·002 ± 0·030	1·928 ± 0·020	99·4
O(2)	Mo	O(3)	2·128 ± 0·030	2·058 ± 0·010	77·9
O(2)	Mo	O(4)	2·128 ± 0·030	1·928 ± 0·020	90·4
O(3)	Mo	O(3)	2·058 ± 0·010	2·058 ± 0·010	79·8
O(3)	Mo	O(4)	2·058 ± 0·010	1·928 ± 0·020	166·7
O(4)	Mo	O(4)	1·928 ± 0·020	1·928 ± 0·020	95·1
Mo	Mo	Mo	2·524 ± 0·002	3·235 ± 0·002	120
Tetrahedral zinc					
O(2)	Zn(1)	O(3)	1·986 ± 0·030	1·978 ± 0·010	114·4
O(3)	Zn(1)	O(3)	1·978 ± 0·010	1·978 ± 0·010	104·1
Octahedral zinc					
O(4)	Zn(2)	O(4)	2·072 ± 0·020	2·072 ± 0·020	89·3
O(3)	Zn(2)	O(3)	2·123 ± 0·010	2·123 ± 0·010	76·9
O(3)	Zn(2)	O(4)	2·123 ± 0·010	2·072 ± 0·020	96·6

* Standard deviations for bond lengths were estimated by formula $\sigma(l)=[\sigma^2(A)+\sigma^2(B)]^{\frac{1}{2}}$, which assumes isotropic standard deviations.

† Estimated standard errors for angles are about 1°.

Table 3. *Observed and calculated structure factors*

H	K	L	FOBS	FCAL
1	0	0	15	12
2	0	0	104	104
3	0	0	27	10
4	0	0	72	73
5	0	0	65	63
6	0	0	98	102
7	0	0	59	55
8	0	0	11	0
9	0	0	15	7
10	0	0	28	29
11	0	0	24	27
1	1	0	42	38
2	1	0	60	55
3	1	0	8	3
4	1	0	34	27
5	1	0	42	38
6	1	0	18	13
7	1	0	47	45
8	1	0	31	25
9	1	0	10	9
2	2	0	204	216
3	2	0	54	52
4	2	0	42	41
5	2	0	7	3
6	2	0	35	38
7	2	0	47	41
8	2	0	31	36
9	2	0	32	31
10	2	0	19	13
3	3	0	58	55
4	3	0	55	48
5	3	0	27	20
6	3	0	15	10
7	3	0	26	27
8	3	0	9	6
9	3	0	46	39
4	4	0	79	76
5	4	0	43	37
6	4	0	13	8
7	4	0	9	5
8	4	0	16	19
5	5	0	60	59
6	5	0	23	20
7	5	0	18	22
8	5	0	13	0
6	6	0	25	17
7	6	0	23	14
1	0	1	29	28
2	0	1	125	133
3	0	1	77	75
4	0	1	75	77
5	0	1	66	64
6	0	1	24	15
7	0	1	14	2
8	0	1	25	24
9	0	1	50	50
10	0	1	23	10
11	0	1	31	25
2	1	1	49	49
3	1	1	5	2
4	1	1	49	46
5	1	1	10	2
6	1	1	18	14
7	1	1	22	16
8	1	1	9	3
9	1	1	25	20
10	1	1	9	5
3	2	1	11	3
4	2	1	50	55
5	2	1	69	66
6	2	1	19	17
7	2	1	47	42
8	2	1	20	21
9	2	1	10	4
10	2	1	10	10
4	3	1	39	38
5	3	1	32	28
6	3	1	39	32
7	3	1	28	26
8	3	1	10	2
9	3	1	0	3
5	4	1	12	1
6	4	1	9	13
7	4	1	40	35
8	4	1	9	4
6	5	1	23	20
7	5	1	34	32
8	5	1	14	7
7	6	1	9	4
0	0	2	130	124
1	0	2	104	97
2	0	2	66	61
3	0	2	116	118
4	0	2	34	33
5	0	2	25	21
6	0	2	17	15
7	0	2	82	85
8	0	2	12	21
9	0	2	41	45
10	0	2	10	13
11	0	2	17	14
1	1	2	129	128
2	1	2	16	14
3	1	2	53	50
4	1	2	71	69
5	1	2	8	4
6	1	2	46	43
7	1	2	17	13
8	1	2	13	6
9	1	2	10	6
10	1	2	13	10
2	2	2	60	60
3	2	2	100	99
4	2	2	14	12
5	2	2	68	70
6	2	2	13	14
7	2	2	24	19
8	2	2	10	12
9	2	2	48	47
10	2	2	32	26
3	3	2	35	33
4	3	2	22	14
5	3	2	15	7
6	3	2	35	39
7	3	2	7	9
4	4	2	16	7
5	4	2	64	62
6	4	2	13	11
7	4	2	39	38
8	4	2	9	5
5	5	2	22	16
6	5	2	9	5
7	5	2	12	8
6	6	2	22	13
7	6	2	32	26
1	0	3	86	80
2	0	3	113	117
3	0	3	64	63
4	0	3	62	60
5	0	3	99	100
6	0	3	16	13
7	0	3	13	14
8	0	3	15	16
9	0	3	41	43
10	0	3	28	20
11	0	3	45	34
2	1	3	100	100
3	1	3	37	35
4	1	3	42	40
5	1	3	28	28
6	1	3	8	6
7	1	3	19	13
8	1	3	22	20
9	1	3	14	8
3	2	3	27	27
4	2	3	40	41
5	2	3	61	58
6	2	3	12	10
7	2	3	61	65
8	2	3	22	19
9	2	3	9	7
4	3	3	68	67
5	3	3	16	9
6	3	3	35	28
7	3	3	8	10
8	3	3	0	9
9	3	3	15	3
5	4	3	12	13
6	4	3	9	7
7	4	3	35	29
8	4	3	22	14
6	5	3	38	39
7	5	3	22	20
8	5	3	18	7
0	0	4	147	156
1	0	4	29	31
2	0	4	107	108
3	0	4	31	29
4	0	4	72	72
5	0	4	52	49
6	0	4	47	50
7	0	4	66	63
8	0	4	9	5
9	0	4	12	15
10	0	4	22	25
11	0	4	23	23
1	1	4	35	32
2	1	4	39	36
3	1	4	13	10
4	1	4	21	20
5	1	4	34	31
6	1	4	25	19
7	1	4	33	30
8	1	4	28	22
9	1	4	10	9
10	1	4	17	13
2	2	4	101	105
3	2	4	60	61
4	2	4	41	40
5	2	4	23	20
6	2	4	34	35
7	2	4	34	33
8	2	4	14	12
9	2	4	35	35
10	2	4	13	17
3	3	4	33	35
4	3	4	36	38
5	3	4	17	18
6	3	4	13	11
7	3	4	24	27
4	4	4	34	35
5	4	4	45	43
6	4	4	0	7
7	4	4	15	13
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5	5	4	45	42
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7	5	4	19	18
6	6	4	12	11
7	6	4	19	17
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4	0	5	114	114
5	0	5	55	53
6	0	5	17	12
7	0	5	27	23
8	0	5	39	46
9	0	5	45	39
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11	0	5	26	18
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3	1	5	38	35
4	1	5	38	36
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6	1	5	36	33
7	1	5	17	12
8	1	5	0	11
9	1	5	31	30
3	2	5	35	33
4	2	5	83	86
5	2	5	56	53
6	2	5	40	40
7	2	5	41	39
8	2	5	18	17
9	2	5	0	12
10	2	5	18	16
4	3	5	32	30
5	3	5	44	43
6	3	5	31	25
7	3	5	32	34
5	4	5	20	19
6	4	5	0	32
7	4	5	30	28
6	5	5	21	18
7	5	5	40	38
0	0	6	115	119
1	0	6	63	62
2	0	6	64	63
3	0	6	58	57
4	0	6	43	43
5	0	6	37	26
6	0	6	32	30
7	0	6	73	70
8	0	6	27	17
9	0	6	29	24
10	0	6	9	19
11	0	6	16	18
1	1	6	51	50
2	1	6	5	6
3	1	6	33	30
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5	1	6	14	12
6	1	6	36	31
7	1	6	9	11
8	1	6	9	12
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3	2	6	75	75
4	2	6	25	23
5	2	6	40	38
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7	2	6	22	22
8	2	6	10	7
9	2	6	41	37
3	3	6	12	8
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5	3	6	11	6
6	3	6	13	17
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5	4	6	53	50
6	5	6	10	8
7	5	6	13	13
6	6	6	9	5
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2	0	7	66	69
3	0	7	55	52
4	0	7	38	40
5	0	7	83	85
6	0	7	18	12
7	0	7	29	29
8	0	7	16	14
9	0	7	43	42
10	0	7	22	23
2	1	7	83	82
3	1	7	44	44
4	1	7	38	36
5	1	7	32	32
6	1	7	24	24
7	1	7	13	13
8	1	7	14	20
9	1	7	10	13
10	1	7	9	5
3	2	7	38	42
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5	2	7	57	54
6	2	7	17	11
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8	2	7	10	18
9	2	7	11	13
4	3	7	57	59
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7	3	7	16	15
6	4	7	10	9
7	4	7	28	29
8	4	7	20	17
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4	0	8	32	33
5	0	8	32	30
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3	1	8	19	20
4	1	8	21	23
5	1	8	16	13
6	1	8	30	26
7	1	8	13	10
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3	2	8	61	61
4	2	8	17	15
5	2	8	35	37
6	2	8	13	18
3	3	8	10	5
4	3	8	27	23
5	3	8	8	3
4	4	8	31	33
1	0	9	47	42
2	0	9	96	98
3	0	9	49	49
4	0	9	67	67
5	0	9	46	49
6	0	9	9	12
7	0	9	21	21
2	1	9	44	44
3	1	9	33	34
4	1	9	35	34
5	1	9	26	26
6	1	9	26	27
3	2	9	31	30
4	2	9	50	52
5	2	9	56	54
6	2	9	21	24
4	3	9	36	34
5	3	9	32	33
0	0	10	131	126
1	0	10	27	24
2	0	10	56	55
3	0	10	38	38
4	0	10	45	44
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4	4	10	32	34
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2	0	11	76	77
3	0	11	41	40
4	0	11	54	54
5	0	11	67	61
2	1	11	53	51
3	1	11	25	24
4	1	11	31	29
5	1	11	22	22
6	1	11	9	14
3	2	11	21	20
4	2	11	42	44
5	2	11	49	46
4	3	11	42	42
0	0	12	83	80
1	0	12	39	36
2	0	12	42	43
3	0	12	38	37
4	0	12	35	35
5	0	12	31	29
6	0	12	26	27
1	1	12	34	35
2	1	12	22	21
3	1	12	25	23
4	1	12	26	26
5	1	12	20	18
2	2	12	52	56
3	2	12	54	53
3	3	12	20	21
1	0	13	25	22
2	0	13	67	71
3	0	13	37	32
4	0	13	53	50
5	0	13	54	54
2	1	13	38	37
3	1	13	9	13
4	1	13	28	23
3	2	13	13	12
4	2	13	37	39
0	0	14	76	68
1	0	14	40	38
2	0	14	34	31
3	0	14	41	43
4	0	14	26	26
1	1	14	41	42
2	1	14	19	19
3	1	14	27	27
4	1	14	30	31
2	2	14	49	50
3	2	14	49	53
2	0	15	60	60
3	0	15	31	30
4	0	15	42	42
2	1	15	28	28
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0	0	0	0	0
0	0	0	0	0
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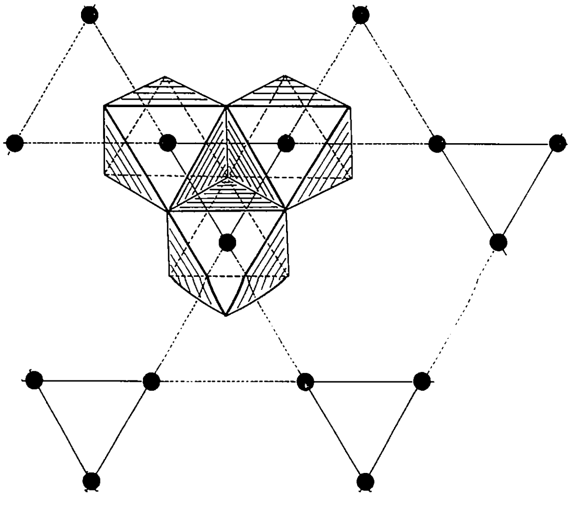

Fig. 1. Pattern of a layer of molybdenum ions (black circles). The molybdenum ions lie in strings with alternating long and short separations. Oxygen coordination is shown around one triangular, bonded grouping of molybdenums. The *c* axis is normal to the plane of the drawing.

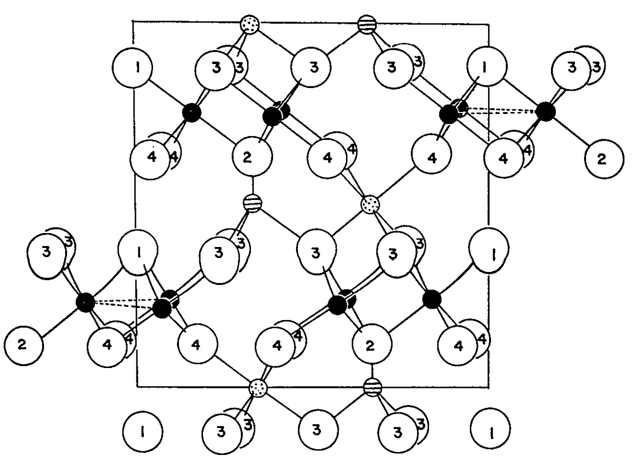

Fig. 2. Bonding scheme in $Zn_2Mo_3O_8$. Large circles are oxygen atoms, numbered as in Tables 1 and 2; black circles are molybdenum ions, striped circles are zinc ions in tetrahedral sites, spotted circles are zinc ions in octahedral sides. The rectangle represents the (110) section of the unit cell, *c* axis vertical. Atomic positions are idealized.

anisotropic refinement). Since the results from all of the refinements were quite close, the fact that the standard errors for the isotropic group *A* refinement were the smallest was the deciding factor in listing the group *A* parameters in Table 1 and calculating from them the bond lengths and angles given in Table 2. The observed and calculated structure factors presented in Table 3 were obtained from the complete, anisotropic, refinement.

Discussion

The essential structural features of the original proposal of McCarroll, Katz & Ward (1957) were found to be correct. The structure consists of a distorted double-hexagonal closest packing (*abcb*) of oxygen atoms in which the oxygen layers are held together by alternate layers of zinc and molybdenum ions. Half of the zinc ions are in approximately tetrahedral coordination with oxygen; the other half are in approximately octahedral coordination. The molybdenum ions are in approximately octahedral coordination with oxygen with the octahedra sharing edges. The molybdenum ions lie in rows with alternately long and short spacings. The rows are arranged with threefold symmetry giving a pattern of molybdenum triangles. Fig. 1 shows this pattern of molybdenum ions and the edge sharing oxygen octahedra about one of the bonded groups (Mo–Mo distance = 2·52 Å). Fig. 2 shows the bonding scheme in the structure in more detail. Oxygen atoms in Fig. 2 are numbered as in Tables 1 and 2.

A final remark on the observed data: the 220 reflection, the one with the largest calculated structure factor, had an observed *F* too small by a factor of almost two in the original work; the new observed value agrees well with the calculated value.

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The Crystal Structure of Sodium Naphthionate Tetrahydrate

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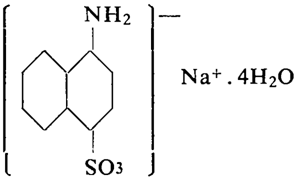
Three-dimensional X-ray diffraction data and electronic computing have been used to determine the positional and thermal atomic parameters in crystalline sodium naphthionate tetrahydrate. 2293 structure amplitudes were used, resulting in $R = 10{\cdot}1\,\%$. The sodium ion is coordinated approximately octahedrally to six oxygen atoms, with a mean Na–O length of 2·424 Å. In the anion the distances are S–O 1·454, S–C 1·765, and C–N 1·411 Å, while in the aromatic ring, four C–C have mean distance 1·366 Å and the other seven C–C 1·420 Å, similar to the values found in naphthalene.

Introduction

Sodium naphthionate



is of importance as an intermediate in dyestuffs manufacture, and as the crystal structures of relatively few metal-organic compounds were known in 1945 when this work was commenced, it was chosen as the first substance in this class to be investigated. The unit-cell dimensions and space groups of a number of related compounds have already been published (Corbridge, Brown & Wallwork, 1966), and a paper describing the structure of this substance was presented at the Glasgow Conference of the X-Ray Analysis Group (*Brit. J. Appl. Phys.* 1961). Other structure determinations of metal salts of organic sulphonic acids include zinc and

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