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The Crystal Structure of Tutton's Salts.
V. Manganese Ammonium Sulfate Hexahydrate

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The crystal structure of manganese ammonium sulfate hexahydrate, $Mn(NH_4)_2(SO_4)_2 . 6H_2O$, has been determined by a three-dimensional X-ray analysis with Fe $K\alpha$ radiation ($\lambda = 1{\cdot}9373$ Å). The crystals are monoclinic, space group $P2_1/a$, with 2 molecules per unit cell. The cell dimensions are $a = 9{\cdot}40$, $b = 12{\cdot}74$, $c = 6{\cdot}26$ Å, $\beta = 107°$. The water molecules are arranged about the manganese ion in an almost regular octahedron, the average metal–oxygen distance being 2·18 Å

Introduction

As a part of a comparative study of the isomorphous series of Tutton's salts (Montgomery & Lingafelter, 1964*a*, 1964*b*, 1966*a*, 1966*b*) we have determined the crystal structure of manganese(II) ammonium sulfate hexahydrate, $Mn(NH_4)_2(SO_4)_2 . 6H_2O$.

Experimental

The procedure followed was essentially that for the isomorphous zinc salt (Montgomery & Lingafelter, 1964*a*). Because of the very great absorption of Cu $K\alpha$ radiation by manganese, the radiation used for intensity measurements was Fe $K\alpha$ ($\lambda = 1{\cdot}9373$ Å). The cell dimensions were measured from rotation and zero-level ($hk0$) Weissenberg photographs (calibrated with sodium chloride, $a_0 = 5{\cdot}6387$ Å) taken with copper radiation ($\lambda = 1{\cdot}5418$ Å) and a precession photograph (Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å) of the a^*c^* net. The results and their estimated standard deviations are $a = 9{\cdot}398 \pm 0{\cdot}015$, $b = 12{\cdot}742 \pm 0{\cdot}020$, $c = 6{\cdot}256 \pm 0{\cdot}006$ Å, $\beta = 106°59' \pm 6'$. Systematic absences, $h0l$ when h is odd, $0k0$ when k is odd, indicate the space group $P2_1/a$, $Z = 2$.

Intensities were recorded by multiple-film technique for the levels $hk0$ through $hk3$ on a Nonius Weissenberg camera, integrating in one direction only, and were measured by a photometer. The raw intensities were corrected for Lorentz and polarization factors and for absorption ($\mu = 91$ cm^{-1}, $\mu R = 0{\cdot}591$) by Bond's (1959) method. The resulting structure factors were then scaled by levels to correspond to the calculated values, using the parameters of the zinc salt. (It should be noted that this scaling procedure precludes physical interpretation of the anisotropic thermal parameters). In all, 554 reflections were surveyed, of which 56 were below minimum observed intensities and 11 were given zero weight in refinements because of secondary extinction effects. The intensities of the remainder varied from 1 to 2730.

The atomic parameters of the heavy atoms were taken from the isomorphous zinc salt and those for hydrogen from the magnesium salt (Montgomery & Lingafelter, 1964*b*). Scattering factors for the manganese ion were taken from Thomas & Umeda (1957); for sulfur from Viervoll & Øgrim (1949); for oxygen and nitrogen from Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955); and for hydrogen from McWeeny (1951). The scattering factor for the Mn ion was modified to allow for the large dispersion effect for iron radiation, $\Delta f' = -4{\cdot}1$, $\Delta f'' = 0$. (James, 1948). The refinement was carried out by least-squares, first in isotropic and then in anisotropic mode, where the anisotropic temperature factor was of the form

$$\exp\{-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)\}.$$

The calculations were carried out on an IBM 7094 computer with programs developed at the University of Washington (Stewart, 1964). A modified Hughes weighting scheme was used with $\sqrt{w} = 0$ for unobserved reflections for which $F_c \le F_{\min}$, $\sqrt{w} = 1$ for unobserved reflections for which $F_c > F_{\min}$ and for observed reflections for which $F_o \le 8$, and $\sqrt{w} = 8/F_o$ for observed reflections for which $F_o > 8$, and the function minimized was $\Sigma\, w(F_o - F_c)^2$. The hydrogen atom positions were not refined. (Because of the close agreement between cell dimensions and heavy atom fractional coordinates of the manganese and magnesium salts it is felt that the refined hydrogen coordinates from the magnesium salt are as valid as recalculated assumed positions for the manganese salt. All distances and angles involving hydrogen atoms appear to be reasonable). An average isotropic temperature factor ($B = 2{\cdot}5$) was used for the hydrogen atoms in all calculations. After two cycles of isotropic and two of anisotropic refinement the average shift of position parameters was $0{\cdot}15\sigma$ with a maximum of $0{\cdot}49\sigma$. The corresponding values for the temperature factors were $0{\cdot}20\sigma$ and $0{\cdot}53\sigma$. After a cycle of refinement on level scaling factors and a

Table 1. *Parameters* (*with least-squares standard errors in parentheses*)

Atom	Fractional positional parameters × 10^4			Anisotropic thermal parameters × 10^4					
	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Mn	0	0	0	49 (3)	35 (1)	192 (14)	−2 (1)	15 (4)	3 (3)
S	4069 (2)	1377 (1)	7402 (4)	42 (2)	31 (1)	129 (15)	−5 (1)	17 (4)	−5 (3)
O(3)	4069 (5)	2271 (4)	5907 (10)	157 (8)	44 (3)	265 (30)	−25 (4)	59 (11)	−9 (7)
O(4)	5466 (5)	812 (4)	7842 (10)	65 (6)	75 (4)	352 (31)	12 (4)	14 (10)	−22 (8)
O(5)	2825 (4)	674 (3)	6294 (8)	65 (6)	43 (3)	217 (30)	−9 (3)	37 (9)	−8 (6)
O(6)	3870 (5)	1766 (4)	9495 (11)	98 (6)	48 (3)	248 (34)	−10 (4)	46 (10)	−6 (9)
O(7)	1774 (5)	1088 (3)	1718 (9)	92 (6)	54 (4)	212 (29)	−22 (3)	39 (9)	−1 (7)
O(8)	−1671 (4)	1150 (3)	325 (9)	53 (5)	38 (3)	351 (27)	0 (3)	33 (9)	−8 (7)
O(9)	−16 (4)	−726 (3)	3096 (9)	97 (6)	41 (3)	254 (30)	12 (3)	62 (10)	10 (7)
N	1331 (6)	3507 (4)	3592 (11)	89 (7)	50 (4)	237 (37)	8 (4)	50 (12)	13 (8)

Table 2. *Observed and calculated structure factors*

Columns are k, $10F_o$ and $10F_c$. Unobserved reflections are marked with *, and those omitted because of secondary extinction are marked with *E*.

0,K,0		
2	384	341
4	748E	-894
6	65	-54
8	296	280
10	37*	-11
12	64	67
1,K,0		
2	375	-400
3	749E	1004
4	43	-41
5	35	18
6	105	-95
7	34*	-4
8	36*	17
9	216	208
10	36*	-4
11	295	300
12	109	108
2,K,0		
0	471	545
1	519	573
2	233	238
3	150	-174
4	298	326
5	180	-182
6	230	237
7	35*	4
8	124	123
9	203	200
10	35*	35
11	31*	6
12	125	115
3,K,0		
1	309	343
2	162	-156
3	244	259
4	502	535
5	463	493
6	141	132
7	122	116
8	151	-136
9	147	-146
10	244	-237
11	61	44
12	103	104
4,K,0		
0	171	-170
1	223	248
2	633E	743
3	204	-194
4	483	502
5	308	-304
6	225	-214
7	53	-35
8	174	-173
9	233	227
10	235	217
11	49	42
5,K,0		
1	578	662
2	110	-104
3	365	-360
4	65	62
5	60	46
6	111	101
7	392	382
8	62	-56
9	218	200
10	91	-88
6,K,0		
0	74	69
1	182	-178
2	366	365
3	37*	-27
4	173	161
5	80	78
6	57	-43
7	59	54
8	37	28
9	23*	7
7,K,0		
1	419	429
2	304	324
3	68	66
4	85	-68
5	49	-50
6	101	-99
7	58	55
8	66	61
8,K,0		
0	123	116
1	296	-274
2	68	65
3	172	-161
4	164	157
5	111	109
6	184	184
9,K,0		
1	36	-31
2	234	252
0,K,1		
0	298	336
1	527	573
2	384	346
3	476	442
4	96	-89
5	238	232
6	403	406
7	28*	9
8	249	253
9	31*	31
10	302	297
11	186	-180
12	65	63
1,K,1		
1	504E	662
2	386	-390
3	89	-97
4	353	394
5	262	273
6	259	261
7	346	354
8	165	-151
9	205	203
10	124	-120
11	161	-162
-1,K,1		
1	119	121
2	549	-565
3	479	462
4	210	-205
5	112	105
6	205	202
7	143	143
8	154	155
9	446	433
10	279	-255
11	155	152
12	128	117
2,K,1		
0	562E	-686
1	479E	632
2	508E	625
3	477	552
4	644E	762
5	377	-400
6	53	52
7	43	-39
8	206	-199
9	31*	-2
10	240	251
11	24*	11
12	215	222
-2,K,1		
0	782E	1131
1	253	288
2	107	120
3	278	292
4	70	-66
5	344	342
6	465	474
7	317	-316
8	282	269
9	31*	9
10	125	-116
11	25*	-21
12	37	33
3,K,1		
1	28	19
2	144	156
3	141	-123
4	166	167
5	484	540
6	30*	-36
7	507	537
8	180	-184
9	130	115
10	141	127
11	82	-78
-3,K,1		
1	304	-349
2	456	539
3	772E	964
4	182	187
5	482	511
6	76	-73
7	189	-186
8	40	41
9	31*	-25
10	148	-138
11	394	365
12	16*	11
4,K,1		
0	128	130
1	148	-144
2	351	381
3	284	283
4	331	331
5	266	266
6	99	-83
7	109	99
8	62	57
9	247	-244
10	177	170
11	111	-109
-4,K,1		
0	44	-36
1	92	96
2	152	-150
3	235	247
4	340	344
5	227	232
6	461	472
7	99	-100
8	476	466
9	172	-159
10	83	-87
11	20*	-6
5,K,1		
1	272	277
2	281	286
3	132	118
4	154	-160
5	103	92
6	65	-55
7	157	169
8	137	124
9	130	116
10	46	51
-5,K,1		
1	375	404
2	139	133
3	156	142
4	160	-146
5	114	104
6	213	-205
7	137	122
8	102	95
9	26*	24
10	187	172
11	210	209
6,K,1		
0	439	474
1	378	-409
2	76	71
3	238	-250
4	30*	-34
5	292	280
6	125	118
7	56	50
8	258	256
-6,K,1		
0	165	176
1	188	-178
2	226	230
3	31*	-29
4	236	222
5	253	229
6	54	-35
7	213	208
8	175	155
9	285	-257
10	198	191
7,K,1		
1	160	-139
2	341	354
3	301	299
4	25*	37
5	207	199
6	100	-94
7	83	73
-7,K,1		
1	397	398
2	233	223
3	156	-139
4	138	138
5	46	-34
6	35	-33
7	362	338
8	36	-24
-8,K,1		
0	307	-289
1	72	-57
2	86	75
3	26*	-26
4	396	377
5	22*	-0
6	167	153
-9,K,1		
1	181	173
2	25	10
3	74	66
4	68	60
0,K,2		
0	189	-192
1	260	-260
2	52	-46
3	288	-284
4	634	663
5	347	-340
6	311	311
7	242	240
8	43	47
9	38*	32
10	269	270
11	29*	-14
12	120	127
1,K,2		
1	96	99
2	31	-19
3	156	143
4	32	-39
5	142	137
6	219	-216
7	508	530
8	39*	-17
9	185	188
10	263	266
11	27*	-2
-1,K,2		
1	799E	931
2	718	-773
3	54	-25
4	250	-244
5	201	-189
6	425	435
7	343	355
8	54	-47
9	195	198
10	51	-44
11	131	-128
12	21*	-6
2,K,2		
0	155	152
1	171	178
2	77	39
3	215	212
4	448	454
5	186	189
6	213	197
7	58	-53
8	166	165
9	259	-270
10	50	48
11	55	46
-2,K,2		
1	172	-194
2	177	197
3	206	207
4	445	485
5	161	-167
6	371	387
7	37*	-14
8	80	74
9	209	207
10	252	263
11	43	-41
12	101	103
3,K,2		
1	175	183
2	229	218
3	310	309
4	256	-261
5	205	211
6	430	-445
7	46	36
8	206	200
9	32*	18
10	255	252
-3,K,2		
1	88	84
2	76	77
3	166	181
4	193	-197
5	369	384
6	73	68
7	156	156
8	138	-139
9	200	212
10	85	-85
11	63	67
4,K,2		
0	179	169
1	220	-230
2	76	79
3	313	-303
4	40	36
5	282	272
6	239	241
7	36*	4
8	372	366
9	130	-122
10	18*	16
-4,K,2		
0	37	31
1	83	79
2	283	311
3	31*	-0
4	63	62
5	276	-280
6	359	367
7	280	-293
8	249	246
9	280	287
10	53	-50
11	174	181
5,K,2		
1	75	-68
2	145	-132
3	257	246
4	130	-125
5	300	302
6	71	66
7	47	40
8	181	173
9	86	89
-5,K,2		
1	49	55
2	74	79
3	363	380
4	119	110
5	357	366
6	39*	7
7	188	-184
8	36*	7
9	97	91
10	97	-97
6,K,2		
4	107	-81
5	30*	-6
6	164	146
-6,K,2		
0	281	287
1	52	-49
2	57	41
3	349	-342
4	153	-150
5	38*	37
6	311	314
7	141	133
8	452	471
9	29	22
-7,K,2		
1	38*	21
2	136	-126
3	239	234
4	37*	-39
5	188	178
6	123	-117
8	107	101
-8,K,2		
0	238	240
1	140	-137
2	110	102
3	228	-234
4	122	119
5	99	91
6	46	42
7	104	110
-9,K,2		
1	41	41
2	264	271
3	57	54
4	52	52
0,K,3		
0	637	680
1	128	-129
2	218	213
3	482	-426
4	67	63
5	347	333
6	205	200
7	137	140
8	48	38
9	201	-211
1,K,3		
1	367	384
2	299	283
3	366	356
4	24*	4
5	90	86
6	455	-458
7	205	-207
8	100	101
9	99	93
10	175	185
-1,K,3		
1	179	170
2	52	46
3	449	396
4	70	75
5	24*	17
6	85	-86
7	184	188
8	193	186
9	115	111
10	22*	-5
11	36	35
2,K,3		
0	198	208
1	111	106
2	250	242
3	92	-90
4	142	-142
5	50	-51
6	248	247
7	54	-45
8	322	348
9	21*	-19
-2,K,3		
0	277	290
1	366	-353
2	59	60
3	533	-524
4	516	487
5	24*	3
6	58	59
7	113	117
8	96	-89
9	39	31
10	185	190
11	22	17
3,K,3		
1	270	274
2	39	-39
3	194	197
4	88	88
5	201	203
6	75	74
7	166	-177
8	45	-50
9	35	37
-3,K,3		
1	636	675
2	146	140
3	59	52
4	47	-33
5	156	-154
6	27*	13
7	300	291
8	81	-82
9	24*	-4
10	20*	-12
11	57	-54
4,K,3		
0	151	149
1	27*	30
2	278	262
3	59	51
4	59	59
5	190	-195
6	80	90
7	42	27
8	94	107
-4,K,3		
0	110	101
1	79	77
2	336	331
3	375	361
4	419	413
5	196	-197
6	183	-194
7	171	-170
8	48	-54
9	148	145
10	242	249
5,K,3		
1	149	149
2	392	-407
3	123	127
4	115	-107
5	122	127
6	252	271
-5,K,3		
1	275	272
2	25*	-10
3	105	-106
4	27*	-15
5	162	167
6	161	151
7	322	320
8	167	-168
9	66	71
10	62	-61
6,K,3		
0	20*	12
1	93	95
2	59	63
3	169	170
4	174	180
-6,K,3		
0	258	264
1	41	-37
2	324	326
3	68	-65
4	34	42
5	275	-289
6	25*	-12
7	23*	8
8	63	66
9	167	188
-7,K,3		
1	81	79
2	277	-287
3	262	275
4	25*	32
5	199	206
6	217	218
7	137	-150
8	23	-24

Table 3. *Bond lengths and angles*

With estimated standard deviations in parentheses for each bond type.

Mn–O(7)(H_2O)	2·193 (0·006)	O(7)–Mn–O(8)	89·7 (0·2)
Mn–O(8)(H_2O)	2·200	O(7)–Mn–O(9)	92·0
Mn–O(9)(H_2O)	2·150	O(8)–Mn–O(9)	90·6
S—O(3)	1·475 (0·007)	O(3)–S—O(4)	109·6 (0·3)
S—O(4)	1·452	O(3)–S—O(5)	108·5
S—O(5)	1·475	O(3)–S—O(6)	109·3
S—O(6)	1·462	O(4)–S—O(5)	109·7
		O(4)–S—O(6)	110·1
		O(5)–S—O(6)	109·6

Table 4. *Hydrogen-bond distances*

Bond	Relative position of second atom*			Bond length (Å)
O(7)—O(5)	x	y	z	2·792 (0·015)
O(7)—O(6)	x	y	$z-1$	2·856
O(8)—O(4)	$x-1$	y	$z-1$	2·720
O(8)—O(6)	$x-\frac{1}{2}$	$\frac{1}{2}-y$	$z-1$	2·781
O(9)—O(3)	$\frac{1}{2}-x$	$y-\frac{1}{2}$	$1-z$	2·715
O(9)—O(5)	$-x$	$-y$	$1-z$	2·776
N(10)–O(3)	x	y	z	3·004 (0·020)
N(10)–O(3)	$x-\frac{1}{2}$	$\frac{1}{2}-y$	z	3·065
N(10)–O(4)	$x-\frac{1}{2}$	$\frac{1}{2}-y$	z	3·112
N(10)–O(5)	$\frac{1}{2}-x$	$\frac{1}{2}+y$	$1-z$	2·869
N(10)–O(6)	$x-\frac{1}{2}$	$\frac{1}{2}-y$	$z-1$	2·929

* This is the transformation relating each 'second atom' to the corresponding atom in the original asymmetric unit.

final F_c calculation, the R index ($R=\Sigma\,||F_o|-|F_c||/\Sigma\,|F_o|$, omitting unobserved reflections and those exhibiting secondary extinction effects) was 0·051. The parameters are listed in Table 1, the observed and calculated structure factors in Table 2, bond lengths and angles in Table 3 and hydrogen-bond distances in Table 4.

Discussion

The main point of interest is the arrangement of water molecules about the manganese ion. The Mn–O distances show the same pattern as in the other Tutton salts (with the exception of copper); two equatorial bonds of 2·19 and 2·20 Å and a shorter axial bond of 2·15 Å. These bond lengths are in agreement with previously recorded Mn–O bond lengths in $MnCl_2.4H_2O$ (Zalkin, Forrester & Templeton, 1964) of 2·206 Å (averaged).

The general packing of the ions and the hydrogen-bond network is essentially identical with that found in the other Tutton's salts, that is, each water molecule forms two hydrogen-bonds (Table 4) which range in length from 2·72 to 2·86 Å. The ammonium ion is also hydrogen-bonded to the oxygen atoms of the sulfate groups, but one bond (to O(3) and O(4) of the same sulfate ion) is 'bifurcated'. In addition, there is a fairly close approach of the water octahedra along the *c* axis, the O(9)–O(9′) distance being 3·009 Å.

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Crystallographic Data for Cerium–Zinc Compounds[*]

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Nine compounds were identified in the cerium–zinc system. The X-ray data obtained for CeZn and $CeZn_{11}$ are consistent with previously reported structures. The compound $CeZn_5$ is shown to be isostructural with $CaCu_5$ as previously reported but the lattice constants $a=5\cdot4163$ to $5\cdot4069$ Å and $c=4\cdot2647$ to $4\cdot2757$ Å, which correspond to the composition range $CeZn_{5\cdot36}$ to $CeZn_{5\cdot10}$ respectively, are significantly different. The unit cells and diffraction symmetries for all the remaining compounds except $CeZn_7$ were determined. Orthorhombic $CeZn_2$, $a=4\cdot63$, $b=7\cdot54$, $c=7\cdot50$ Å, is isostructural with $CeCu_2$. $CeZn_3$ and Ce_3Zn_{11} are also found to be orthorhombic with $a=4\cdot62$, $b=10\cdot43$, $c=6\cdot64$ Å for $CeZn_3$ and $a=4\cdot5215$, $b=8\cdot8855$, $c=13\cdot463$ Å for Ce_3Zn_{11}. $CeZn_{4\cdot5}$ is hexagonal with $a=14\cdot60$, $c=14\cdot11$ Å. Ce_2Zn_{17} is shown to be isostructural with U_2Zn_{17}, space group $R\bar{3}m$. Only X-ray data on powdered specimens of $CeZn_7$ were obtained.

Introduction

In a study of the cerium–zinc alloy system, X-ray diffraction data along with thermal, metallographic and vapor pressure data were employed to establish the phase diagram. The purpose of this paper is to summarize the X-ray diffraction data obtained; the other data have been reported elsewhere (Chiotti & Mason, 1965).

There are nine compounds in this system; six, $CeZn_3$, $CeZn_{3\cdot67}$, $CeZn_{4\cdot5}$, $CeZn_{5\cdot25}$, $CeZn_7$ and $CeZn_{11}$ decompose peritectically at 820, 840, 870, 885, 960 and 795°C respectively, and three, CeZn, $CeZn_2$ and $CeZn_{8\cdot5}$ melt congruently at 825, 875 and 980°C respectively.

X-ray work on three of the nine compounds has been reported by earlier investigators. Iandelli & Botti (1937) showed that the compound CeZn has the CsCl structure, space group $Pm3m$, with $a=3\cdot704$ Å. Sanderson & Baenziger (1953) determined the structure of $BaCd_{11}$ from single crystal data. They compared powder diffraction data of this compound with powder diffraction data for $CeZn_{11}$, $LaZn_{11}$, $PrZn_{11}$ and $SrCd_{11}$ and found that all of them give patterns with similar line spacings and relative intensities and suggest they are isostructural with $BaCd_{11}$. The lattice constants for

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