and its molecular conformation is transplanar (Damiani, Giglio, Puliti & Ripamonti, 1965). Both spermine and spermidine interact with deoxyribonucleic acid (DNA) in solution, as inferred by the increased helix coil transition temperature of the macromolecule and by the electrochemical behaviour (Liquori and coworkers, to be published).

Such a strong affinity may be readily explained if a skewed conformation is assumed which allows a stereospecific interaction leading to a cross linking of the DNA strands in the narrow groove of the double helix.

Model studies indicate that a conversion from the *B* structure to the *A* structure is likely to be thus induced. These considerations which will be developed in more detail elsewhere appear to support a stereochemical model for the ribonucleic acid synthesis on a DNA template, proposed by one of us (Liquori, to be published), which appears to be accelerated in the presence of spermine and spermidine (Weiss & Fox, 1964).

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The Crystal Structure of Tutton's Salts. III. Copper Ammonium Sulfate Hexahydrate

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The crystal structure of copper ammonium sulfate hexahydrate, $Cu(NH_4)_2(SO_4)_2 . 6H_2O$, has been determined by a three-dimensional X-ray analysis, using Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å). The crystals are monoclinic, space group $P2_1/a$, 2 molecules per cell. The cell dimensions are:

$$a = 9{\cdot}27, \quad b = 12{\cdot}44, \quad c = 6{\cdot}30 \text{ Å}, \quad \beta = 106{\cdot}1^\circ.$$

The water molecules are arranged about the copper ion in an octahedron which shows orthorhombic distortion, the three metal–oxygen bond distances being 2·22, 2·10, and 1·96 Å.

Introduction

In a continuing study (Montgomery & Lingafelter, 1964*b*) of the structures of an isomorphous series of hydrated double sulfates (Tutton's salts), one of the primary points of interest was the behavior of the copper(II) ion. In general, this ion exhibits a 4+2 arrangement of ligands when there are six present, and it was expected that the copper salt would show a coordination configuration of the water molecules about the central ion which would differ from the general pattern of the rest of the series. In support of this expectation, it was noted that the angle β for the copper salt is about one degree less than the average for the series. This salt was, therefore, one of the first to be examined when the general structure of the Tutton's salts had been established.

Experimental

The procedure followed was essentially that for the isomorphous zinc salt (Montgomery & Lingafelter, 1964*a*) except that the crystal needle was ground to approximate a cylinder (along **c**) ($\mu = 59{\cdot}16$ cm^{-1}, $\mu R = 0{\cdot}31$). The cell dimensions (calibrated with $a_0 = 5{\cdot}6387$ Å for NaCl) were found to be: $a = 9{\cdot}267 \pm 0{\cdot}02$, $b = 12{\cdot}445 \pm 0{\cdot}015$, $c = 6{\cdot}298 \pm 0{\cdot}005$ Å, $\beta = 106^\circ 9' \pm 6'$. Systematic absences, $h0l$ when h is odd, $0k0$ when k is odd – space group $P2_1/a$, $Z = 2$.

The raw intensities were collected by photometric measurements of singly integrated equi-inclination Weissenberg photographs taken about the c axis ($hk0$ through $hk4$) and were corrected for Lorentz and polarization factors and for absorption after Bond's (1959) method, and converted to structure factors. The resulting structure factors were then scaled by levels to correspond to the calculated values, using the parameters from the isomorphous zinc salt (Montgomery & Lingafelter, 1964*a*). In all, 1119 reflections were used, of which 120 were below minimum observed values, and 12 were omitted from all calculations because of secondary extinction effects.

The initial parameters were taken from the isomorphous zinc salt for the heavy atoms and from the magnesium salt (Montgomery & Lingafelter, 1964*b*) for the hydrogen atoms. Refinement was by full-matrix 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 computer programs used were those developed at the University of Washington (Stewart, 1964).

Scattering factors were from Thomas & Umeda (1957) for the copper ion, from Viervoll & Øgrim (1949) for sulfur, from Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for oxygen and nitrogen and from McWeeny (1951) for hydrogen. A modified Hughes weighting scheme was used, and the function minimized was $\Sigma w(F_o-F_c)^2$. No great accuracy can be claimed for the hydrogen atom positions, which were allowed to vary for four cycles in the least-squares refinement, and an average isotropic temper-

Table 1. *Final atomic parameters*

		x/a	$\sigma_x\times10^4$	y/b	$\sigma_y\times10^4$	z/c	$\sigma_z\times10^4$
	Cu(1)	0·000		0·000		0·000	
	S(2)	0·4089	0·9	0·1394	0·6	0·7458	1·9
	O(3)	0·4150	3·4	0·2320	2·3	0·6003	5·9
	O(4)	0·5479	3·3	0·0763	2·5	0·7818	6·6
	O(5)	0·2801	2·9	0·0702	1·9	0·6331	5·5
	O(6)	0·3905	3·6	0·1779	2·3	0·9566	6·1
	O(7)	0·1751	3·2	0·1151	2·5	0·1775	5·7
	O(8)	−0·1644	3·0	0·1096	2·1	0·0321	5·9
	O(9)	−0·0053	2·9	−0·0642	2·0	0·2820	5·7
	N(10)	0·1335	3·9	0·3477	2·7	0·3599	7·3
N	H(11)	0·075	68	0·313	52	0·203	111
	H(12)	0·191	70	0·299	50	0·368	110
	H(13)	0·082	68	0·335	48	0·454	105
	H(14)	0·155	67	0·395	48	0·342	108
O(7)	H(15)	0·196	69	0·082	47	0·277	122
	H(16)	0·242	69	0·131	47	0·131	110
O(8)	H(17)	−0·250	70	0·097	46	−0·076	106
	H(18)	−0·153	70	0·167	50	−0·003	106
O(9)	H(19)	−0·104	66	−0·057	50	0·308	109
	H(20)	0·004	68	−0·132	48	0·310	102

Table 2. *Anisotropic temperature parameters and their standard deviations*

(a) Anisotropic temperature parameters ($\times 10^2$)

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cu(1)	0·594	0·344	1·85	−0·006	0·280	0·050
S(2)	0·403	0·239	1·37	−0·050	0·194	−0·044
O(3)	1·15	0·322	1·86	−0·191	0·489	0·006
O(4)	0·568	0·553	3·18	0·091	0·220	−0·239
O(5)	0·607	0·350	1·59	−0·146	0·339	−0·066
O(6)	1·09	0·406	1·53	−0·050	0·387	−0·111
O(7)	0·755	0·546	1·68	−0·007	0·337	0·152
O(8)	0·691	0·337	2·30	−0·058	0·273	0·150
O(9)	0·645	0·321	1·76	0·058	0·416	0·100
N(10)	0·755	0·400	2·26	0·027	0·409	0·087

(b) Standard deviation of temperature factors ($\times 10^4$)

Cu(1)	1·0	0·5	5·0	0·4	1·4	0·7
S (2)	1·1	0·6	5·8	0·5	1·6	0·9
O(3)	4·3	1·7	14·4	2·0	5·2	3·1
O(4)	3·5	2·2	16·7	2·1	5·2	4·1
O(5)	3·2	1·7	12·6	1·7	4·3	3·2
O(6)	4·1	1·9	14·0	2·1	5·0	3·4
O(7)	3·7	1·9	14·3	2·1	4·9	3·7
O(8)	3·3	1·7	13·7	1·8	4·6	3·3
O(9)	3·1	1·5	13·0	1·7	4·4	3·1
N(10)	4·4	2·2	18·9	2·2	6·2	4·0

Table 3. *Observed and calculated structure factors* (x10)

Columns are k, $10F_o$ and $10F_c$. Unobserved reflections are marked * and extinctions with an E.

k	10Fo	10Fc
	0,K,0	
2	398	484
4	579	-640
6	83	92
8	354	352
10	39*	-9
12	168	171
14	280	306
	1,K,0	
1	154	194
2	361	-399
3	760E	1186
4	25	-16
5	164	154
6	48	-43
7	107	121
8	34*	-31
9	309	319
10	39*	-25
11	355	359
12	137	140
13	37*	-14
14	33*	36
15	68	60
	2,K,0	
0	507E	762
1	450	526
2	338	392
3	173	-166
4	477	555
5	171	-156
6	353	363
7	45	-44
8	213	199
9	191	188
10	49	49
11	40*	-17
12	170	167
13	80	-86
14	230	227
15	24*	6
	3,K,0	
1	390	461
2	165	-150
3	383	418
4	488	532
5	533	629
6	145	139
7	234	243
8	189	-173
9	97	-83
10	248	-245
11	119	113
12	121	127
13	248	263
14	29*	27
15	175	170
	4,K,0	
0	32	-20
1	314	306
2	647E	864
3	268	-259
4	548	640
5	374	-366
6	115	-92
7	48	-50
8	86	-79
9	316	314
10	249	271
11	41	32
12	194	194
13	117	-94
14	130	125
	5,K,0	
1	626E	777
2	182	-164
3	240	-220
4	93	74
5	215	197
6	100	96
7	466	484
8	40*	-36
9	230	217
10	83	-82
11	39	-37
12	87	79
13	176	169
	6,K,0	
0	131	136
1	143	-131
2	473	503
3	66	-51
4	256	262
5	44	48
6	71	63
7	40*	25
8	91	86
9	39*	7
10	294	317
11	34*	-5
12	120	123
	7,K,0	
1	487	566
2	291	280
3	141	145
4	66	-56
5	40*	31
6	80	-75
7	118	106
8	57	52
9	159	158
10	33*	21
11	28*	16
12	82	-83
	8,K,0	
0	181	175
1	276	-306
2	201	191
3	171	-166
4	240	230
5	111	104
6	227	240
7	37*	4
8	34*	39
9	135	-124
10	77	58
11	138	128
	9,K,0	
1	77	67
2	260	261
3	320	334
4	76	-67
5	188	192
6	141	-140
7	31*	4
8	82	87
9	86	77
	10,K,0	
0	269	291
1	89	-81
2	95	94
3	31*	-14
4	60	60
5	94	86
6	205	193
	11,K,0	
1	172	151
2	59	-53
3	232	222
	0,K,1	
1	519	552
2	496	542
3	466	457
4	29	29
5	359	338
6	511	502
7	51	49
8	316	311
9	77	51
10	394	415
11	255	-252
12	128	130
13	212	-215
14	28*	-5
15	86	91
	1,K,1	
1	590E	835
2	404	-391
3	78	83
4	459	451
5	325	335
6	300	290
7	432	415
8	213	-174
9	296	296
10	165	-134
11	34*	-29
12	63	65
13	272	280
14	27*	9
15	139	140
	-1,K,1	
1	257	316
2	512	-550
3	552	626
4	253	-252
5	209	188
6	281	247
7	275	257
8	204	194
9	513	534
10	229	-213
11	230	232
12	122	129
13	64	69
14	28*	-0
15	22*	6
	2,K,1	
0	449	-500
1	535E	678
2	640E	850
3	505	537
4	704	838
5	356	-362
6	131	133
7	33	36
8	164	-151
9	45	26
10	370	383
11	34*	-11
12	288	285
13	41	-37
	-2,K,1	
0	801E	1307
1	291	278
2	210	222
3	256	238
4	20*	25
5	351	359
6	573	615
7	277	-248
8	407	385
9	145	128
10	34*	-34
11	79	-75
12	128	131
13	163	-157
14	280	287
15	44	43
	3,K,1	
1	164	188
2	117	109
3	60	-24
4	272	222
5	601	667
6	34	-32
7	588	655
8	137	-140
9	204	199
10	151	151
11	56	-54
12	71	-65
13	170	184
14	41	-43
15	150	157
	-3,K,1	
1	188	-160
2	475	537
3	797E	1100
4	185	176
5	539	582
6	63	-48
7	147	-123
8	74	66
9	114	98
10	138	-136
11	445	459
12	33*	9
13	88	93
14	81	-87
	4,K,1	
0	205	231
1	122	-100
2	482	540
3	316	326
4	435	425
5	259	275
6	32	39
7	158	145
8	129	115
9	235	-243
10	232	227
11	88	-94
12	208	215
13	76*	25
14	83	77
	-4,K,1	
0	103	97
1	129	135
2	71	-46
3	281	259
4	443	478
5	329	311
6	535	579
7	104	-98
8	531	582
9	181	-167
10	34*	-26
11	34*	-26
12	53	50
13	41	39
14	206	212
	5,K,1	
1	414	429
2	303	283
3	169	170
4	152	-142
5	191	178
6	33*	-16
7	256	252
8	160	150
9	207	208
10	49	53
11	142	150
12	232	-229
13	49	43
	-5,K,1	
1	463	490
2	153	128
3	288	275
4	109	-93
5	245	235
6	178	-173
7	191	189
8	123	117
9	109	95
10	141	143
11	315	316
12	102	-109
13	69	74
14	56	-56
	6,K,1	
0	500	565
1	422	-456
2	213	207
3	219	-222
4	97	88
5	318	299
6	151	140
7	79	83
8	277	288
9	156	-156
10	108	110
11	27*	24
12	116	119
	-6,K,1	
0	296	289
1	211	-198
2	303	306
3	36	-33
4	316	323
5	297	261
6	33*	18
7	215	216
8	292	291
9	273	-268
10	272	275
11	65	-61
12	71	71
13	89	86
	7,K,1	
1	34*	-18
2	359	381
3	359	369
4	34*	27
5	258	255
6	57	-56
7	117	125
8	73	76
9	146	161
10	27	-27
11	218	226
	-7,K,1	
1	484	509
2	266	260
3	62	-51
4	129	129
5	55	48
6	45	-37
7	411	418
8	37	24
9	171	173
10	31	37
11	46	45
12	228	-220
	8,K,1	
0	412	449
1	55	45
2	135	133
3	78	77
4	69	71
5	85	82
6	191	194
7	66	-62
8	154	151
	-8,K,1	
0	200	-194
1	84	-83
2	153	151
3	34*	-18
4	422	443
5	34*	-6
6	207	204
7	80	77
8	55	57
9	45	-51
10	262	265
11	20*	18
	9,K,1	
1	31*	32
2	31*	0
3	307	309
4	117	116
5	169	172
6	25*	24
7	23*	-1
8	86	-81
	-9,K,1	
1	235	242
2	34*	29
3	125	121
4	67	68
5	127	132
6	51	51
7	196	210
8	63	-65
9	102	78
	-10,K,1	
0	30*	6
1	100	119
2	120	137
3	111	128
4	213	215
5	101	-92
6	186	176
7	21*	-16
	-11,K,1	
1	80	71
2	89	-89
3	122	119
4	138	119
5	118	117
	0,K,2	
0	203	-158
1	261	-233
2	63	69
3	230	-206
4	732	757
5	365	-347
6	397	401
7	284	264
8	179	178
9	31*	-10
10	351	457
11	33*	-18
12	233	233
13	39	44
14	127	-132
	1,K,2	
1	205	135
2	39	37
3	262	277
4	38	35
5	247	250
6	234	-220
7	574	611
8	89	-69
9	311	309
10	238	240
11	92	94
12	84	-89
13	90	91
14	24*	-20
15	143	157
	-1,K,2	
1	776E	1018
2	684	-769
3	68	77
4	213	-200
5	97	-63
6	445	436
7	499	471
8	112	-37
9	319	298
10	82	-74
11	33*	-22
12	32*	4
13	275	271
14	95	86
15	203	200
	2,K,2	
0	228	256
1	208	216
2	92	95
3	318	335
4	526	560
5	196	184
6	298	296
7	78	-64
8	300	302
9	334	-334
10	172	163
11	47	47
12	180	190
13	162	179
14	77	77
	-2,K,2	
0	411	-402
1	176	-190
2	275	289
3	263	236
4	526	533
5	231	-203
6	552	551
7	27*	-9
8	237	236
9	212	192
10	381	397
11	71	-70
12	122	133
13	182	-188
14	47	-38
15	81	89
	3,K,2	
1	260	278
2	281	266
3	349	358
4	263	-257
5	312	293
6	455	-455
7	203	197
8	194	188
9	151	138
10	245	257
11	266	289
12	81	-78
13	59	53
14	53	-52
	-3,K,2	
1	163	169
2	125	115
3	270	298
4	185	-174
5	482	521
6	102	81
7	329	313
8	180	-175
9	294	305
10	114	-99
11	122	122
12	217	223
13	160	170
14	76	74
15	38	32
	4,K,2	
0	242	242
1	244	-245
2	109	119
3	287	-290
4	175	174
5	331	338
6	345	338
7	32*	-0
8	464	434
9	161	-160
10	68	68
11	29*	5
12	26*	33
13	110	108
	-4,K,2	
0	108	113
1	103	78
2	361	395
3	26	21
4	133	131
5	317	-307
6	476	570
7	317	-317
8	363	352
9	298	293
10	78	75
11	172	173
12	77	76
13	97	-82
14	207	209
	5,K,2	
1	24*	-5
2	86	-76
3	332	317
4	131	-122
5	361	388
6	34	37
7	145	141
8	171	174
9	179	176
10	81	-89
11	259	287
12	38	-48
	-5,K,2	
1	144	146
2	130	123
3	477	514
4	164	156
5	429	444
6	30*	20
7	146	-133
8	72	-66
9	228	224
10	132	-138
11	362	369
12	70	68
13	69	67
	6,K,2	
0	392	412
1	54	55
2	254	243
3	33*	5
4	33*	5
5	49	53
6	201	201
7	43	-44
8	233	237
9	51	50
10	88	79
11	89	-76
12	39	40
	-6,K,2	
0	353	361
1	27*	-17
2	160	151
3	309	-321
4	65	-66
5	46	48
6	413	430
7	78	68
8	483	542
9	33*	1
10	55	55
11	29*	-36
12	26	26
13	49	48
	7,K,2	
1	33*	21
2	205	-203
3	248	251
4	32*	-21
5	233	235
6	49	49
7	91	101
8	76	-79
9	172	176
10	26*	-28
	-7,K,2	
1	85	84
2	133	-136
3	320	303
4	56	-38
5	293	287
6	118	-115
7	115	118
8	117	117
9	213	210
10	50	50
11	244	250
12	74	-65
	8,K,2	
0	133	135
1	270	232
2	123	125
3	176	179
4	78	80
5	203	-204
6	184	209
7	80	-80
8	142	137
9	140	143
	-8,K,2	
0	323	339
1	132	-128
2	178	182
3	272	-279
4	165	171
5	91	81
6	117	104
7	81	84
8	177	175
9	90	-98
10	111	120
11	33	36
	9,K,2	
1	87	87
2	100	-99
3	93	82
4	105	103
5	144	137
6	95	94
	-9,K,2	
1	122	118
2	265	271
3	107	101
4	56	41
5	150	173
6	151	-193
7	283	310
8	40	44
9	94	90
10	76	76
	10,K,2	
0	40	32
1	17*	14
2	135	138
	-10,K,2	
0	65	-57
1	93	-92
2	94	94
3	58	-57
4	311	336
5	26*	20
6	93	86
7	57	-44
8	38	34
	-11,K,2	
1	171	163
2	23*	14
3	22*	7
4	80	-80
5	77	77
	0,K,3	
0	633E	803
1	175	-149
2	282	294
3	489	-498
4	248	243
5	276	278
6	278	281
7	69	53
8	115	106
9	209	-198
10	105	89
11	43	39
12	185	191
13	162	171
14	124	128
	1,K,3	
1	428	492
2	274	278
3	471	489
4	88	-82
5	171	162
6	484	-531
7	91	-77
8	145	138
9	199	187
10	204	204
11	251	257
12	30	-28
13	92	93
14	39	-41
	-1,K,3	
1	266	257
2	22	12
3	521	556
4	18*	1
5	167	169
6	117	-85
7	329	315
8	199	189
9	198	177
10	30*	-33
11	74	70
12	150	-165
13	116	114
14	27	-26
	2,K,3	
0	288	290
1	113	98
2	303	309
3	189	-188
4	36	-31
5	49	-36
6	390	409
7	105	-97
8	419	466
9	37	-42
10	60	61
11	127	130
12	33	-34
13	104	111
14	165	168
	-2,K,3	
0	334	363
1	395	-419
2	143	146
3	555	-600
4	626	673
5	75	-66
6	206	197
7	102	81
8	28*	33
9	64	62
10	234	237
11	63	55
12	227	241
13	63	69
14	19*	-9
	3,K,3	
1	320	346
2	55	-54
3	295	290
4	91	86
5	324	336
6	28*	-9
7	70	-71
8	72	-67
9	107	102
10	37	-34
11	238	254
12	49	51
13	116	115
	-3,K,3	
1	585E	756
2	51	44
3	129	133
4	116	-104
5	22*	26
6	24*	20
7	453	461
8	102	-87
9	52	47
10	29*	-8
11	37	-35
12	99	97
13	178	186
14	17*	9
	4,K,3	
0	205	180
1	28	23
2	334	358
3	35	-32
4	116	120
5	208	-207
6	228	224
7	30*	30
8	197	196
9	143	147
10	26*	25
11	46	-48
12	28	28
	-4,K,3	
0	234	261
1	71	69
2	416	455
3	343	355
4	495	532
5	292	-286
6	123	-112
7	197	-195
8	61	55
9	151	147
10	310	302
11	83	78
12	175	174
13	93	-92
14	21	26
	5,K,3	
1	201	194
2	408	-447
3	225	238
4	140	-137
5	251	251
6	222	226
7	52	46
8	75	-76
9	77	79
10	40	-50
11	141	137
	-5,K,3	
1	358	359
2	22*	-4
3	23*	20
4	25*	-15
5	286	294
6	143	125
7	392	420
8	196	-214
9	141	134
10	53	-52
11	86	79
12	130	139
13	94	79
	6,K,3	
0	77	71
1	89	84
2	151	146
3	150	157
4	213	218
5	193	-190
6	177	187
7	26*	-29
8	110	113
9	149	142
10	136	132
	-6,K,3	
0	329	359
1	59	-56
2	411	432
3	72	-63
4	173	159
5	329	-351
6	87	79
7	29*	7
8	129	122
9	196	190
10	118	111
11	55	54
12	118	104
13	79	-76
	7,K,3	
1	283	308
2	42	-49
3	77	77
4	28	-32
5	25*	2
6	43	41
7	165	172
8	74	-72
9	100	112
	-7,K,3	
1	159	159
2	321	-321
3	376	386
4	29*	-9
5	288	286
6	205	204
7	85	-80
8	28*	-38
9	108	108
10	66	-72
11	194	211
	8,K,3	
0	109	110
1	24*	-6
2	110	136
3	32	31
4	193	213
5	48	-41
6	17*	20
7	73	-65
	-8,K,3	
0	431	477
1	29*	38
2	234	230
3	30*	-22
4	96	-96
5	29*	-39
6	262	280
7	46	46
8	190	199
9	23*	-13
10	20*	-26
11	53	-52
	9,K,3	
1	152	151
2	16*	21
3	14*	14
	-9,K,3	
1	29*	-0
2	46	-36
3	317	344
4	70	-62
5	195	232
6	124	-116
7	24*	-24
8	22*	18
9	164	157
	-10,K,3	
0	366	373
1	26*	-5
2	156	190
3	53	-39
4	24*	2
5	56	51
6	132	122
7	65	-60
8	85	79
	-11,K,3	
1	160	149
2	166	158
3	141	125
4	48	-41
5	85	83
	0,K,4	
0	496	489
1	91	77
2	339	312
3	104	95
4	77	-65
5	83	-82
6	346	333
7	107	95
8	267	265
9	37	-29
10	83	74
11	18	-20
12	46	40
13	32	-25
	1,K,4	
1	367	367
2	21	16
3	287	264
4	345	346
5	201	171
6	155	159
7	25	13
8	244	-244
9	172	170
10	45	-54
11	187	205
12	14*	-11
13	65	60
	-1,K,4	
1	7*	-2
2	92	93
3	606	582
4	57	-56
5	400	393
6	83	-75
7	73	-67
8	141	127
9	174	168
10	54	55
11	178	171
12	151	-138
13	133	136
14	5*	-18
	2,K,4	
0	473	504
1	214	200
2	350	354
3	200	167
4	59	53
5	376	-371
6	40	24
7	42	46
8	225	213
9	161	166
10	95	94
11	15*	-17
12	65	62
	-2,K,4	
1	249	-261
2	404	404
3	207	-185
4	81	81
5	421	399
6	334	305
7	52	46
8	47	-37
9	201	-194
10	19*	11
11	23	-27
12	161	182
13	66	65
	3,K,4	
1	241	229
2	231	-223
3	155	151
4	131	113
5	223	220
6	247	243
7	192	190
8	180	-180
9	54	49
10	81	-88
11	118	116
12	80	87
	-3,K,4	
1	125	117
2	441	436
3	395	360
4	26	20
5	283	282
6	139	-124
7	173	170
8	178	186
9	213	222
10	53	-52
11	61	58
12	132	-152
13	95	97
	4,K,4	
0	41	-39
1	40	39
2	159	153
3	95	101
4	414	425
5	64	-66
6	80	90
7	18*	6
8	41	41
9	96	106
10	94	101
11	58	-62
	-4,K,4	
0	318	303
1	35	-27
2	326	314
3	38	-33
4	237	218
5	283	274
6	118	108
7	138	-138
8	151	146
9	115	-111
10	188	202
11	16*	20
12	135	132
13	72	78
	5,K,4	
1	311	322
2	76	77
3	92	92
4	18*	7
5	68	57
6	65	66
7	145	179
8	15*	11
9	13*	-4
10	89	-93
	-5,K,4	
1	541	577
2	114	120
3	67	-59
4	25	-24
5	56	49
6	117	-118
7	337	344
8	59	56
9	129	129
10	17*	21
11	15*	17
12	39	39
13	82	91
	6,K,4	
0	73	71
1	92	-99
2	142	137
3	80	-84
4	250	256
5	91	90
6	32	28
7	50	-45
8	11*	5
	-6,K,4	
0	78	84
1	202	193
2	342	346
3	182	186
4	452	464
5	59	62
6	136	-140
7	19*	-13
8	19*	7
9	18*	-9
10	211	223
11	104	-108
12	164	167
	7,K,4	
1	229	239
2	178	174
3	26	26
4	35	-28
5	12*	-14
6	101	-103
	-7,K,4	
1	265	247
2	200	-203
3	19*	9
4	99	96
5	197	206
6	152	161
7	318	352
8	45	-50
9	41	26
10	92	-90
11	47	47
	8,K,4	
0	116	124
1	52	-48
2	107	102
3	24	-27
	-8,K,4	
0	66	67
1	108	111
2	155	158
3	74	76
4	322	330
5	127	-139
6	90	92
7	50	59
8	59	54
9	74	79
10	90	85
	-9,K,4	
1	180	180
2	122	-160
3	223	239
4	64	61
5	76	79
6	123	134
7	23	20
8	81	-75
9	61	62
	-10,K,4	
0	315	345
1	95	118
2	82	82
3	214	206
4	48	-48
5	27	-27
6	199	204
	-11,K,4	
1	29	20
2	42	36
3	239	248

ature factor ($B=2·6$) was used in the calculation of their contribution to structure factors. The final R index was 0·060 ($R=\Sigma||F_o|-|F_c||/\Sigma|F_o|$ with omission of unobserved reflections and those suffering from secondary extinction). During the final cycle, all parameters of non-hydrogen atoms shifted less than 0·1σ. For the hydrogen atoms, the mean shift was 0·24σ and the maximum was 1·1σ. The final parameters are listed in Tables 1 and 2, the observed and calculated structure factors in Table 3, bond lengths and angles in Table 4 (together with the estimated standard deviations calculated from the final least-squares refinement), and hydrogen bond distances in Table 5.

Table 4. *Bond lengths and angles*

Estimated standard deviation in parentheses for each bond type

Bond lengths (Å)		Bond angles (°)	
Cu–H_2O [O(7)]	2·219 (0·005)	O(7)–Cu–O(8)	88·89 (0·15)
Cu–H_2O [O(8)]	2·095	O(7)–Cu–O(9)	90·35
Cu–H_2O [O(9)]	1·961	O(8)–Cu–O(9)	88·61
S–O(3)	1·484 (0·005)	O(3)–S–O(4)	109·14 (0·2)
S–O(4)	1·471	O(3)–S–O(5)	108·62
S–O(5)	1·482	O(3)–S–O(6)	109·85
S–O(6)	1·466	O(4)–S–O(5)	108·56
		O(4)–S–O(6)	110·63
		O(5)–S–O(6)	110·00

Table 5. *Hydrogen bond distances*

	Relative position of second atom*			Bond length (Å)
O(7)—O(5)	x	y	z	2·818 (0·010)
O(7)—O(6)	x	y	$z-1$	2·841
O(8)—O(4)	$x-1$	y	$z-1$	2·725
O(8)—O(6)	$x-\frac{1}{2}$	$\frac{1}{2}-y$	$z-1$	2·759
O(9)—O(3)	$\frac{1}{2}-x$	$y-\frac{1}{2}$	$1-z$	2·709
O(9)—O(5)	$-x$	$-y$	$1-z$	2·745
N(10)-O(3)	x	y	z	2·996 (0·015)
N(10)-O(3)	$x-\frac{1}{2}$	$\frac{1}{2}-y$	z	3·013
N(10)-O(4)	$x-\frac{1}{2}$	$\frac{1}{2}-y$	z	3·123
N(10)-O(5)	$\frac{1}{2}-x$	$\frac{1}{2}+y$	$1-z$	2·879
N(10)-O(6)	$x-\frac{1}{2}$	$\frac{1}{2}-y$	$z-1$	2·906

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

Discussion

The main point of interest is the arrangement of the water molecules about the central copper ion. The bond lengths of 2·22, 2·10 and 1·96 Å break the pattern of the other Tutton salts, as expected, but do not exhibit the tetragonally distorted octahedral arrangement commonly associated with the Cu(II) ion. Instead the distortion is orthorhombic, the Cu–O(7) bond being roughly the average of the two extremes. A similar pattern is shown in the copper perchlorate hexahydrate where the bond lengths are reported to be 2·28, 2·16, 2·09 Å (Mani & Ramaseshan, 1961).

The general packing of the ions and the hydrogen bond network is essentially identical with that found in the other Tutton salts. Each water molecule forms two hydrogen bonds (Table 5) which range in length from 2·71 Å to 2·84 Å. The ammonium ion is also hydrogen bonded to oxygen atoms of the sulfate groups. Three of the hydrogen atoms form normal hydrogen bonds, while the fourth, H(13), forms a bifurcated hydrogen bond. The only other close approach of non-bonded atoms is that of the two O(9) atoms 3·16 Å across the center of symmetry at 0,0, $\frac{1}{2}$.

After this work was completed, a report appeared of a two-dimensional study of the same structure (Webb, Kay & Grimes, 1965). A few comparisons may be of interest. The mean difference in positional parameters (x_i/a_i, expressed as multiples of the two-dimensional standard deviation) between the two determinations is 1·0, and just two of these parameters, x of S and z of O(9), differ by more than 2·0. Webb, Kay & Grimes have discussed, at some length, the differences between the hydrogen bond distances in the copper compound and those in the nickel and magnesium compounds. In fact, the more precise values from our three-dimensional determinations show that there is no significant difference in the range of hydrogen bond lengths. Thus for the Cu salt the OH---O lengths range from 2·71 to 2·84 Å; for Ni, from 2·73 to 2·86 Å; for Zn, from 2·72 to 2·85 Å; and for Mg, from 2·73 to 2·86 Å.

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