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Salt Hydrates. IX. The Comparison of the Crystal Structure of Magnesium Sulfate Pentahydrate with Copper Sulfate Pentahydrate and Magnesium Chromate Pentahydrate

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The salt $MgSO_4.5H_2O$ crystallizes in space group $P\bar{1}$, $Z=2$, $a=6{\cdot}314$ (5), $b=10{\cdot}505$ (18), $c=6{\cdot}030$ (6) Å, $\alpha=81°7$ (12)′, $\beta=109°49$ (12)′, $\gamma=105°5$ (3)′. The crystal structure was refined using three-dimensional X-ray data (precession camera, Mo $K\alpha$ radiation) to $R=0{\cdot}057$ for 1366 observed structure factors. The Mg coordination octahedra and sulfate tetrahedra form chains of composition $Mg(OH_2)_4SO_4$ extending parallel to [110]. The chains are connected to each other by hydrogen bonds, donated by the water oxygen atoms in the chain and by the fifth water molecule, which is not coordinated to an Mg atom. The salt should be formulated as $[Mg(OH_2)_4SO_4].H_2O$. The hydrogen atom positions were determined from difference syntheses and were confirmed by a calculation of the positions of least electrostatic energy. The hydrogen atom positions in $MgCrO_4.5H_2O$ were calculated on the basis of geometrical arguments. $MgSO_4.5H_2O$ is isostructural with $CuSO_4.5H_2O$, this being one of the few cases where a Cu salt and a Mg salt crystallize in the same structure type and in the same space group. The lengths of the hydrogen bonds in all three pentahydrates conform well with the extended electrostatic valence rule, which predicts that hydrogen bonds formed by water molecules bonded to a Cu ion in the square-planar coordination should be shorter than those donated by water molecules bonded to Mg ions. The comparison of the sulfate pentahydrates and of the difluorides of Mg and Cu suggests that the Jahn–Teller effect is not a sufficient condition for explaining the low lattice symmetries of Cu salts as compared with analogous Mg salts.

Introduction

Magnesium sulfate can be crystallized out of aqueous solution as the mono-, five-fourth-, di-, tri-, tetra-, penta-, hexa- and hepta-hydrate (Hodenberg & Kühn, 1967). Only the mono-, the hexa- and the hepta-hydrate, however, are stable in contact with their solutions. Pentahydrate crystals are metastable in contact with an $MgSO_4$ solution at all temperatures, but they can be stored for a prolonged time when separated from their solution and shielded from the atmosphere. Magnesium sulfate pentahydrate has even been reported (Palache, Berman & Frondel, 1951) to occur as a mineral (pentahydrite). Magnesium and divalent copper only rarely form strictly isostructural pairs of compounds; one pair is $MgSO_4.5H_2O$ and $CuSO_4.5H_2O$. By 'strictly isostructural', we mean in this context that two compounds have the same crystal structure and crystallize in the same space group. In many cases, Cu compounds analogous to an Mg compound do not exist (*e.g.* $MgCO_3$ is known, but $CuCO_3$ is not). When an analogous Cu compound does exist, usually either it has a completely different structure from that of the Mg compound, as in the case of CuO and MgO, or at least its crystal structure represents a distortion from the structure of the Mg compound, as in the case of

CuF_2 and MgF_2 (see also Wells, 1962). The structures of CuF_2 and MgF_2 are not strictly isostructural because their symmetries are different even though the coordination numbers around the cations and anions are the same and the topology of the polyhedral connections is identical.

This is a continuation of our previous investigations of salt hydrates (VIII: Khan & Baur, 1972). The refinement part of this work represents a master's thesis of one of the authors (JLR) at the University of Pittsburgh, 1966.

Experimental

Crystals of $MgSO_4.5H_2O$ were grown at 50°C from aqueous solution, which was acidified by the addition of H_2SO_4. The crystals decomposed rapidly after removal from the solution; consequently, they were coated with a thin layer of epoxy resin, which greatly reduced their decomposition rate. A crystal of approximate dimensions $0{\cdot}2 \times 0{\cdot}4 \times 3{\cdot}0$ mm, elongated parallel to the [001] direction and mounted with this zone axis parallel to the spindle axis, was used for data collection on a precession camera. Fourteen layers were recorded by the multiple-exposure technique in directions perpendicular to the c axis, [100], [010], [210], and [210]. About 2400 intensities [$\sin\theta(\max)/\lambda=0{\cdot}85$ Å^{-1}] were estimated visually by comparison with a calibrated strip. The averaging and processing of the data resulted in 1625 unique F_{hkl} data, of which 206 were of zero intensity. The absorption correction was neglected ($\mu(\text{Mo } K\alpha)=5{\cdot}7\,\text{cm}^{-1}, \mu R=0{\cdot}11$ to $0{\cdot}22$). $MgSO_4.5H_2O$ crystallizes in space group $P\overline{1}$. The Mg atoms are in special positions 000 and $\frac{1}{2},\frac{1}{2},0$. All other atoms are in general positions $\pm(x,y,z)$. $Z=2$, F.W. 210·47, $D_x=1{\cdot}93$ g.cm^{-3}, $D_m=1{\cdot}90$ g.cm^{-3} (Hodenberg & Kühn, 1967). For unit-cell data, see Table 1. The cell parameters were derived from a careful measurement of calibrated precession photographs [$\mu(\text{Mo } K\alpha)=0{\cdot}7107$ Å].

Table 1. *Unit-cell data for* $MgSO_4.5H_2O$, $MgCrO_4.5.H_2O$ (*Bertrand et al.*, 1971) *and* $CuSO_4.5H_2O$ (*Bacon & Curry*, 1962)

The values measured for $MgSO_4.5H_2O$ agree with the unit-cell data reported by Hodenberg & Kühn (1967). Estimated standard deviations here and throughout the paper are in parentheses following each value.

	Mg, S salt	Mg, Cr salt	Cu, S salt
a	6·314 (5) Å	6·384 Å	6·141 Å
b	10·565 (18)	10·702	10·736
c	6·030 (6)	6·115	5·986
α	81°7 (12)′	81°33′	82°16′
β	109°49 (12)′	108°45′	107°26′
γ	105°5 (3)′	104°20′	102°40′
V	362·3 Å^3	382·3 Å^3	366·4 Å^3

Starting with the positional parameters reported by Bacon & Curry (1962) for $CuSO_4.5H_2O$, the refinement with isotropic temperature factors and unit weights proceeded to an $R=0{\cdot}123$. At this point, a Hughes-type weighting scheme was introduced, the 14 interlayer scale factors were adjusted, and the data were re-averaged, using the improved scale factors. Refinement with anisotropic temperature factors yielded an $R=0{\cdot}061$. A three-dimensional difference synthesis revealed 10 maxima ranging in height from 0·33 to 0·67 e.Å^{-3}, which were near the expected locations of the hydrogen atoms. The highest background peaks (near the position of the sulfur atom) were 0·4 e.Å^{-3}. The hydrogen atoms were included in the least-squares refinement, with constant isotropic temperature factors equivalent to the observed anisotropic temperature factors of the corresponding oxygen atoms. The R value dropped significantly to 0·057. The 53 F_{obs} data that are believed to be affected by extinction were excluded from refinement. Observed and calculated structure factors are presented in Table 2, the heavy-atom parameters used for the calculation of the final structure factors are listed in Table 3 and the hydrogen-atom parameters are given in Table 4.

Computer programs employed in the course of the work are:

LPFPRE:	Lorentz–polarization factors for the precession camera, Baur, W.H., 1962, unpublished.
ORFLS:	crystallographic least-squares, (Busing, Martin & Levy, 1962) (in a local modification).
FORDAP:	Fourier synthesis (Zalkin, 1962, unpublished) (in a local modification).
ORFFE:	crystallographic function and errors, (Busing, Martin & Levy, 1964) (in a local modification).
SADIAN 69:	Bond distances, bond angles, and structure sketches, (Baur & Wenninger, 1969, unpublished).
MANIOC:	Electrostatic energies of crystals (Baur, 1965).
CALHPO:	Geometrical calculation of hydrogen atom positions (Baur, 1969, unpublished)

Discussion of the structure

The main features of the crystal structure of $MgSO_4.5H_2O$ agree with those of $CuSO_4.5H_2O$ as determined by Beevers & Lipson (1934) and confirmed by neutron diffraction by Bacon & Curry (1962). The two crystallographically different Mg atoms are octahedrally coordinated by four water oxygen atoms and two sulfate oxygen atoms each (Table 5). They share corners with the coordination tetrahedra around the S atoms to form chains of alternating octahedra and tetrahedra extending parallel to [110] (Fig. 1). These chains of composition $Mg(OH_2)_4SO_4$ contain four of the water molecules per formula unit, while the fifth one, O(W9), is not coordinated to a Mg atom. It is held in the structure by hydrogen bonds in an approximately tetrahedral arrangement. Of the ten hydrogen bonds formed by the five crystallographically independent water molecules, four reinforce the $Mg(OH_2)_4SO_4$ chains within themselves, while the six remaining ones connect every chain with its six neighbor-chains (the arrangement of the chains around each other is approximately close-packed). The compound can be formulated, in analogy to the Cu salt, as $[Mg(OH_2)_4SO_4].H_2O$.

Surprisingly, neither Beevers & Lipson (1934), nor Bacon & Curry (1962) have pointed out the chains of octahedra and tetrahedra in $CuSO_4.5H_2O$. They limited their attention to the immediate environments of the atoms. Consequently, this feature has not been

Table 2. $MgSO_4.5H_2O$, *observed and calculated structure factors* (×10)

Values marked with an asterisk were given zero weight in the least-squares refinement.

H	K	L	FO	FC
-9	-4	1	49	49
-8	-4	2	76	80
-8	-4	3	44	39
-8	-3	1	110	113
-8	-3	2	23	22
-8	-3	3	61	54
-6	-4	1	44	44
-6	-4	2	55	58
-6	-4	3	171	172
-6	-4	4	30	32
-6	-3	1	170	170
-6	-3	2	97	93
-6	-3	3	71	70
-6	-3	4	121	123
-6	-3	5	84	75
-6	-2	1	102	99
-6	-2	2	171	176
-6	-2	3	44	35
-6	-2	5	133	128
-6	-1	1	74	67
-6	-1	2	129	132
-6	-1	3	50	44
-6	-1	4	154	148
-6	0	1	119	121
-6	0	2	63	60
-6	0	3	58	57
-6	1	1*	0	31
-6	1	2	41	41
-6	1	3	77	77
-6	2	-5*	0	4
-6	2	0	196	204
-6	2	1	56	55
-6	2	2	52	50
-6	2	3	63	62
-6	2	4	52	51
-6	2	5	55	52
-6	3	0	119	114
-6	3	1	30	29
-6	3	2	139	141
-6	3	3	80	85
-6	3	4	78	82
-6	3	5	45	49
-6	4	0	38	39
-6	4	1	162	167
-6	4	2*	0	12
-6	4	3	52	53
-6	4	4	108	115
-5	-12	1	63	64
-5	-12	2	73	74
-5	-11	1	56	53
-5	-11	2	51	52
-5	-11	3	122	115
-5	-10	1	48	45
-5	-10	2	42	35
-5	-9	1	137	136
-5	-9	2	118	118
-5	-9	3	26	23
-5	-8	1	141	145
-5	-8	2	25	31
-5	-8	3	65	61
-5	-8	4	86	91
-5	-4	1	32	37
-5	-4	2	73	49
-5	-4	3	33	40
-5	-4	4	46	47
-5	-4	6	56	56
-5	-3	1	193	211
-5	-3	2	27	26
-5	-3	4	123	129
-5	-3	5	40	42
-5	-3	6	40	30
-5	-2	2	115	117
-5	-2	3	56	59
-5	-2	5	124	133
-5	-2	6	75	74
-5	-1	1	111	109
-5	-1	3	145	150
-5	-1	4	100	89
-5	0	1	101	103
-5	0	2	25	26
-5	0	3	63	57
-5	0	4	83	77
-5	1	0	79	79
-5	1	1	162	160
-5	1	2	47	55
-5	1	3*	0	14
-5	1	4	136	143
-5	1	5	26	35
-5	2	0	85	84
-5	2	1	123	125
-5	2	2	40	39
-5	2	3	19	22
-5	2	4	111	111
-5	2	5	77	82
-5	3	1	115	118
-5	3	2	79	84
-5	3	3	78	85
-5	3	4	56	54
-5	3	5*	0	7
-5	3	6	59	54
-5	4	-6*	0	8
-5	4	-5*	0	11
-5	4	0	93	83
-5	4	1	31	35
-5	4	2	109	107
-5	4	3	34	41
-5	4	4	65	72
-5	4	5	21	24
-5	8	0	92	92
-5	8	3	75	73
-5	9	0	68	69
-5	9	1	28	29
-4	-10	1	155	149
-4	-10	2*	0	9
-4	-10	3	31	33
-4	-10	4	168	155
-4	-9	1	38	41
-4	-9	2	45	46
-4	-9	3	118	123
-4	-8	1	41	41
-4	-8	2	237	232
-4	-8	3	135	133
-4	-8	4	45	43
-4	-7	1	148	149
-4	-7	2	72	74
-4	-7	3	161	147
-4	-7	4	27	24
-4	-7	5	105	109
-4	-6	1	263	275
-4	-6	2	32	28
-4	-6	3	34	35
-4	-6	4	125	135
-4	-6	5	30	29
-4	-4	1	19	18
-4	-4	2	41	42
-4	-4	3	103	117
-4	-4	4	23	29
-4	-4	6	89	96
-4	-3	2	101	98
-4	-3	3	173	194
-4	-3	4	155	165
-4	-3	5	39	37
-4	-2	1	101	110
-4	-2	2	209	237
-4	-2	3	34	34
-4	-2	5	139	143
-4	-1	1*	256	338
-4	-1	3	46	46
-4	-1	4	109	106
-4	-1	5	122	126
-4	-1	6	45	41
-4	0	1	77	78
-4	0	3	177	166
-4	0	4	145	145
-4	0	5	46	47
-4	1	0	203	234
-4	1	1	101	98
-4	1	2	43	36
-4	1	3*	0	19
-4	1	4	48	56
-4	1	5	57	56
-4	1	6	82	83
-4	2	-8*	0	9
-4	2	-6*	0	24
-4	2	0	123	120
-4	2	1	36	32
-4	2	2	102	94
-4	2	3	142	150
-4	2	4	106	106
-4	2	5	135	139
-4	2	6	19	27
-4	3	0	162	143
-4	3	1	41	35
-4	3	2*	0	11
-4	3	3	59	62
-4	3	4	71	73
-4	3	5	72	75
-4	3	6	46	48
-4	4	0	152	146
-4	4	1	313	323
-4	4	2	52	92
-4	4	3	37	32
-4	4	4	140	140
-4	4	5	51	48
-4	4	6*	0	16
-4	6	1	83	79
-4	6	2	137	141
-4	6	3	58	52
-4	6	4	146	145
-4	6	5	100	87
-4	7	0	100	101
-4	7	1	75	79
-4	7	2	69	83
-4	7	3	73	70
-4	7	4	65	59
-4	8	1	69	91
-4	8	2*	0	13
-4	8	3	34	28
-4	9	0	64	87
-4	9	1	72	74
-4	9	2	41	37
-4	9	3	29	29
-4	10	-7*	0	13
-4	10	1	41	43
-4	10	2*	0	21
-4	10	3	120	117
-3	-8	1	53	49
-3	-8	2	149	147
-3	-8	3*	0	19
-3	-8	4	169	166
-3	-8	5	107	101
-3	-8	6	50	44
-3	-7	1	13	18
-3	-7	2	44	44
-3	-7	3	127	136
-3	-7	4	45	46
-3	-7	5	51	46
-3	-7	6	77	66
-3	-6	1	142	131
-3	-6	2	134	131
-3	-6	3	64	41
-3	-6	4	223	228
-3	-6	5	33	31
-3	-5	2	226	238
-3	-5	3	15	15
-3	-5	4	46	50
-3	-5	5	200	196
-3	-5	6	45	48
-3	-4	1	200	212
-3	-4	2	89	91
-3	-4	3	161	179
-3	-4	4	42	46
-3	-4	5	25	21
-3	-4	6	32	33
-3	-3	1	181	191
-3	-3	2	84	89
-3	-3	3	102	100
-3	-3	4	172	193
-3	-3	6	86	94
-3	-2	1	99	109
-3	-2	2	42	47
-3	-2	3	141	155
-3	-2	4	64	64
-3	-2	6	48	52
-3	-1	2	201	218
-3	-1	3*	258	333
-3	-1	5	89	86
-3	-1	6	102	99
-3	0	1	127	113
-3	0	2	100	98
-3	0	4	29	32
-3	0	5	71	69
-3	0	6	40	36
-3	1	0	82	73
-3	1	1*	353	414
-3	1	2	28	26
-3	1	3*	0	13
-3	1	4	236	238
-3	1	6*	0	19
-3	2	0	125	110
-3	2	1	57	62
-3	2	2	184	195
-3	2	3*	0	4
-3	2	4	40	38
-3	2	5	127	135
-3	2	6	114	112
-3	3	0	246	241
-3	3	1	135	133
-3	3	2	81	82
-3	3	3	100	110
-3	3	4*	0	1
-3	3	5	107	108
-3	3	6	65	70
-3	3	7	46	52
-3	4	0	76	69
-3	4	1	209	204
-3	4	2	42	40
-3	4	4	68	67
-3	4	5	133	132
-3	4	6	77	75
-3	4	7	54	53
-3	5	1	142	138
-3	5	2	248	253
-3	5	4	27	23
-3	5	5	74	73
-3	5	6	74	71
-3	6	0	199	192
-3	6	1	196	183
-3	6	2	28	26
-3	6	3	102	104
-3	6	4	120	118
-3	6	5	40	38
-3	7	-4*	0	0
-3	7	0	263	256
-3	7	1	199	202
-3	7	3	100	99
-3	7	4	60	59
-3	7	5	95	95
-3	8	-1*	0	7
-3	8	0	172	170
-3	8	1	157	161
-3	8	2	41	41
-3	8	3	136	137
-3	8	4	98	102
-3	8	5*	0	7
-2	-14	3	114	115
-2	-13	1	89	93
-2	-13	2	74	76
-2	-13	5	85	83
-2	-12	1	80	77
-2	-12	2	78	71
-2	-12	4	89	95
-2	-12	5	53	54
-2	-11	1	65	58
-2	-11	2	49	48
-2	-11	4	62	63
-2	-11	5	83	93
-2	-10	1	143	144
-2	-10	3	70	71
-2	-10	4	61	52
-2	-10	5	70	69
-2	-10	6	76	64
-2	-9	1	121	113
-2	-9	2	164	169
-2	-9	3	78	91
-2	-9	4	51	56
-2	-8	1	44	49
-2	-8	2	150	171
-2	-8	3	70	73
-2	-8	4	105	117
-2	-8	5	130	142
-2	-8	6	44	45
-2	-7	1	104	103
-2	-7	2	126	135
-2	-7	3	141	171
-2	-7	4	85	105
-2	-7	5	101	107
-2	-7	6	151	147
-2	-6	1*	314	350
-2	-5	1	85	89
-2	-5	2	208	239
-2	-5	3	107	125
-2	-5	5	102	105
-2	-5	6	54	54
-2	-4	1	162	167
-2	-4	2	166	170
-2	-4	3	171	189
-2	-4	4	33	33
-2	-4	5	168	176
-2	-4	6	100	99
-2	-3	1	65	65
-2	-3	2	33	35
-2	-3	3	68	66
-2	-3	4	167	176
-2	-3	5	100	102
-2	-3	6	71	66
-2	-2	1	40	40
-2	-2	2	219	240
-2	-2	3	128	133
-2	-2	4	139	137
-2	-2	5	128	130
-2	-2	6	42	44
-2	-2	7	43	43
-2	-1	1	89	107
-2	-1	2*	322	398
-2	-1	3	121	130
-2	-1	4	179	199
-2	-1	5	71	63
-2	-1	6	66	56
-2	-1	7	46	39
-2	0	2	123	121
-2	0	4	23	25
-2	0	5	121	125
-2	0	6	122	118
-2	0	7	55	51
-2	1	0	167	162
-2	1	2	96	90
-2	1	3*	0	25
-2	1	4	144	158
-2	1	5	89	90
-2	1	6*	0	26
-2	1	7	85	85
-2	2	0	89	78
-2	2	1*	321	590
-2	2	2	175	159
-2	2	3	135	129
-2	2	5	121	125
-2	2	6	52	53
-2	2	7	73	69
-2	3	1	140	148
-2	3	2	73	68
-2	3	3	104	103
-2	3	4	141	147
-2	3	5	63	66
-2	3	6	108	106
-2	3	7	74	71
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2	1	5	26	27
2	1	6	44	38
2	1	7	46	52
2	1	8	61	59
2	2	0*	272	312
2	2	1*	395	619
2	2	2	204	234
2	2	3	29	21
2	2	4	152	154
2	2	5*	0	16
2	2	6	25	25
2	2	7	92	92
2	2	8	76	78
2	3	1	74	78
2	3	3	186	167
2	3	4	223	229
2	3	5	109	113
2	3	6*	0	15
2	3	7	55	59
2	3	8	112	107
2	4	0*	334	374
2	4	1	114	133
2	4	2	259	312
2	4	3	152	161
2	4	4	51	44
2	4	5	39	44
2	4	6	118	130
2	4	7	67	70
2	4	8	34	36
2	5	-4*	0	16
2	5	0	53	47
2	5	2	119	113
2	5	3	103	104
2	5	4*	0	1
2	5	5	188	192
2	5	6	43	50
2	5	7	98	106
2	5	8	47	47
2	6	-6*	0	11
2	6	-5*	0	3
2	6	-4*	256	305
2	6	-3*	0	16
2	6	-2*	0	20
2	6	0	77	62
2	6	1	242	234
2	6	3	50	49
2	6	4	70	77
2	6	5	219	254
2	6	6	24	24
2	6	7	31	36
2	6	8	165	176
2	7	0*	351	399
2	7	1	225	240
2	7	2	185	209
2	7	3	82	86
2	7	4	128	153
2	7	5*	0	18
2	7	6	50	63
2	7	7	82	92
2	8	0	171	177
2	8	1	306	315
2	8	2*	0	22
2	8	3	56	51
2	8	4	188	219
2	8	5*	0	40
2	8	6	126	155
2	8	7	117	132
2	8	8*	0	34
2	9	-5*	0	25
2	9	0	269	274
2	9	1	160	157
2	9	2	87	83
2	9	3	137	150
2	9	4	65	77
2	9	5*	0	45
2	9	6	113	129
2	9	7*	0	14
2	9	8	54	49
2	10	-2*	0	2
2	10	0	141	145
2	10	1	152	147
2	10	2	100	103
2	10	3	145	156
2	10	4	82	90
2	10	5	140	163
2	10	6	92	106
2	10	7*	0	33
2	10	8	53	49
2	11	-3*	0	23
2	11	0	77	73
2	11	1	72	58
2	11	2*	0	27
2	11	3*	0	33
2	11	4*	0	36
2	11	5	73	82
2	11	6	76	74
2	11	7	44	50
2	11	8	67	68
2	12	-3*	0	6
2	12	0	67	59
2	12	1	112	116
2	12	2	48	42
2	12	3*	0	5
2	12	4	118	141
2	12	5*	0	2
2	12	6*	0	25
2	12	7	62	67
2	12	8*	0	19
2	13	-3*	0	26
2	13	1	81	81
2	13	2	41	38
2	13	3*	0	1
2	13	4*	0	42
2	13	5	112	127
2	13	6*	0	11
2	13	7	52	49
2	13	8	36	44
2	14	-4*	0	7
2	14	-2*	0	4
2	14	-1*	0	23
2	14	0	155	161
2	14	3	75	75
2	14	6	53	57
3	-8	2	60	58
3	-8	3	138	145
3	-8	4	58	55
3	-8	5	53	48
3	-8	6	93	99
3	-7	3	134	136
3	-7	5	178	192
3	-7	6	66	66
3	-6	2	140	130
3	-6	4	45	40
3	-6	5	98	98
3	-6	6	59	59
3	-5	-3*	0	10
3	-5	2	221	208
3	-5	3	82	76
3	-5	4	249	250
3	-5	5	96	95
3	-5	6	26	26
3	-5	7	109	100
3	-4	1	146	138
3	-4	2	46	38
3	-4	3	103	100
3	-4	4	175	162
3	-4	5	102	98
3	-4	6	60	61
3	-4	7	102	99
3	-4	8	36	34
3	-3	1	38	37
3	-3	2	20	18
3	-3	3	233	253
3	-3	4	59	55
3	-3	5*	0	6
3	-3	6	170	178
3	-3	7	57	54
3	-3	8*	0	26
3	-2	1	212	222
3	-2	2	26	26
3	-2	3	58	53
3	-2	4	346	354
3	-2	5	125	119
3	-2	6	75	66
3	-2	7	156	153
3	-2	8	77	81
3	-1	1	46	47
3	-1	2	35	41
3	-1	3*	0	13
3	-1	4	115	110
3	-1	5	203	185
3	-1	6*	0	0
3	-1	7*	0	19
3	-1	8	105	98
3	0	-3*	0	28
3	0	0	52	51
3	0	1	67	61
3	0	2	54	52
3	0	4	70	67
3	0	5	161	158
3	0	6*	0	26
3	0	7	62	58
3	0	8	101	88
3	1	-4*	0	8
3	1	0*	234	284
3	1	2	201	208
3	1	3	258	274
3	1	4	202	199
3	1	5*	0	3
3	1	6	63	60
3	1	7	40	35
3	1	8	55	50
3	2	-5*	0	17
3	2	2	16	21
3	2	3	149	159
3	2	4	50	48
3	2	5*	0	4
3	2	6	38	39
3	2	7	19	19
3	2	8	20	26
3	3	-5*	0	1
3	3	0	108	118
3	3	2*	343	431
3	3	3	302	315
3	3	4	53	46
3	3	5	159	147
3	3	6	80	64
3	3	7	56	51
3	3	8	159	157
3	4	0	179	191
3	4	1*	326	358
3	4	3	307	298
3	4	4	227	233
3	4	5	195	195
3	4	6	76	73
3	4	7	36	32
3	4	8	68	69
3	5	-1*	0	8
3	5	0	94	94
3	5	2	37	36
3	5	3	25	27
3	5	5	61	67
3	5	6	89	97
3	5	7	244	252
3	5	8*	0	2
3	6	1	233	226
3	6	2	107	101
3	6	3	210	207
3	6	4	100	99
3	6	5	60	60
3	6	6	88	87
3	6	7	32	27
3	6	8	86	88
3	7	0	258	241
3	7	3	141	129
3	7	4	109	95
3	7	5	199	214
3	7	6	124	131
3	7	7	38	36
3	7	8	82	72
3	8	0	162	126
3	8	2	124	115
3	8	4	181	179
3	8	5	24	29
3	8	6	80	84
3	8	7	56	56
3	8	8	138	136
4	-10	1	59	58
4	-10	2	76	76
4	-10	4	77	85
4	-9	1	57	56
4	-9	2	102	104
4	-9	4	25	25
4	-8	1	172	178
4	-8	2	72	75
4	-8	3	67	69
4	-8	4	124	133
4	-8	5	39	42
4	-7	1	98	96
4	-7	3	46	48
4	-7	4	98	94
4	-7	5	114	109
4	-7	6	27	27
4	-6	1	144	144
4	-6	2	162	160
4	-6	3	31	26
4	-6	4	146	149
4	-6	5	51	49
4	-6	6	88	82
4	-6	7	55	54
4	-4	1	150	134
4	-4	2	251	230
4	-4	3	108	96
4	-4	5	222	198
4	-4	6*	0	20
4	-4	7	99	97
4	-4	8	133	123
4	-3	1	216	198
4	-3	3	284	266
4	-3	4	49	49
4	-3	5	21	28
4	-3	6	76	76
4	-3	7*	0	16
4	-3	8	33	31
4	-2	1	82	81
4	-2	2	234	228
4	-2	3	225	205
4	-2	4	142	130
4	-2	5	97	90
4	-2	7	115	115
4	-1	1	62	55
4	-1	2*	0	19
4	-1	3*	0	20
4	-1	4	128	117
4	-1	5	73	72
4	-1	6	131	117
4	-1	7	28	32
4	-1	8	92	89
4	0	0	319	340
4	0	1	224	231
4	0	2	169	179
4	0	3	234	239
4	0	4	62	60
4	0	5	153	162
4	0	6	136	134
4	0	7*	0	5
4	1	-2*	0	3
4	1	0	67	71
4	1	3	128	121
4	1	4	139	125
4	1	5	125	123
4	1	7	28	34
4	1	8	72	70
4	1	9	54	54
4	2	0	60	57
4	2	2	107	110
4	2	3	51	47
4	2	4*	297	345
4	2	5	31	30
4	2	6	74	78
4	2	7	187	185
4	3	-6*	0	20
4	3	2	159	168
4	3	3	180	187
4	3	4	226	242
4	3	5	227	224
4	3	6*	0	22
4	3	7	126	107
4	3	8	92	80
4	3	9	93	96
4	4	-5*	0	29
4	4	3	221	265
4	4	5	74	67
4	4	6	176	176
4	4	7	59	55
4	4	8*	0	17
4	4	9	98	96
4	6	0	51	51
4	6	1	54	53
4	6	2	103	104
4	6	3	113	102
4	6	4	79	75
4	6	5	220	218
4	6	6	46	40
4	6	7*	0	1
4	6	8	148	138
4	6	9	73	71
4	7	0	194	200
4	7	1	75	69
4	7	3	221	233
4	7	4	108	112
4	7	5	40	37
4	7	6	99	91
4	7	7	51	53
4	7	8	24	22
4	8	0	44	39
4	8	1	129	130
4	8	2	33	29
4	8	3	84	82
4	8	4	169	177
4	8	5	39	36
4	8	6	57	58
4	8	7	56	54
4	9	-4*	0	20
4	9	0	185	172
4	9	4	109	95
4	9	5	31	25
4	9	7	47	43
4	10	0	97	89
4	10	2	221	188
4	10	4	42	41
4	10	5	126	120
4	10	6	43	45
4	10	8	79	76
5	-9	1	30	30
5	-9	2	80	79
5	-9	3	104	100
5	-9	4	126	132
5	-8	-2*	0	15
5	-8	1	43	41
5	-8	3	129	128
5	-8	4	85	83
5	-8	5	54	56
5	-8	6	79	80
5	-4	1	45	35
5	-4	2	58	57
5	-4	3	18	21
5	-4	4	55	54
5	-4	8	41	39
5	-3	1*	0	2
5	-3	4	29	30
5	-3	5	99	98
5	-3	6	73	74
5	-3	7*	0	11
5	-3	8	46	43
5	-3	9	51	51
5	-2	1	51	47
5	-2	2	185	179
5	-2	3	54	50
5	-2	4	119	110
5	-2	5	150	151
5	-2	6	44	40
5	-2	7	98	97
5	-2	8	88	89
5	-1	1	219	219
5	-1	2	235	245
5	-1	4	191	187
5	-1	5	84	79
5	-1	7	84	99
5	-1	8	129	130
5	0	0	65	69
5	0	1	98	91
5	0	2	131	124
5	0	3*	0	21
5	0	4	152	155
5	0	5	127	132
5	0	6	85	78
5	0	7	119	119
5	1	-5*	0	21
5	1	0	307	318
5	1	3	202	216
5	1	4	64	64
5	1	5*	0	6
5	1	6	228	235
5	1	7	76	75
5	1	8	37	38
5	2	0	135	135
5	2	3	138	139
5	2	4	81	87
5	2	5	80	80
5	2	7	108	104
5	2	8	39	42
5	2	9	44	39
5	3	-3*	0	16
5	3	3	35	36
5	3	4	26	26
5	3	5	162	158
5	3	6	59	56
5	3	7*	0	0
5	3	8	103	98
5	3	9	56	59
5	4	3	172	183
5	4	4	93	107
5	4	6	181	184
5	4	7	30	25
5	4	8	64	61
5	4	9	58	51
5	8	0	23	29
5	8	1	68	57
5	8	2	31	27
5	8	3	63	52
5	8	4*	0	13
5	8	5	113	113
5	8	6*	0	20
5	8	7*	0	5
5	8	8	65	63
5	9	1	71	72
5	9	2	155	155
5	9	3	126	119
5	9	4	168	157
5	9	6	38	36
5	9	7	55	54
5	9	8	45	47
5	10	0	44	39
5	10	1	25	22
5	10	2	45	41
5	10	3*	0	9
5	10	4	94	95
5	10	6	57	57
5	11	0	162	168
5	11	2	90	78
5	11	3	202	190
5	11	4	32	33
5	11	5*	0	5
5	11	6	92	99
5	11	7	53	53
5	12	2	70	68
5	12	5	99	99
5	12	6*	0	1
6	-4	1	108	108
6	-4	2	225	228
6	-3	1	89	87
6	-3	2	20	26
6	-3	3	154	133
6	-3	4	193	184
6	-3	5	45	39
6	-3	6	52	49
6	-3	7	40	44
6	-3	8*	0	20
6	-2	1	67	67
6	-2	2	59	63
6	-2	3	115	110
6	-2	4	82	83
6	-2	6	118	121
6	-2	7	90	94
6	-2	8	36	39
6	-1	2	38	44
6	-1	3	216	214
6	-1	4	143	148
6	-1	6	57	51
6	-1	7	90	89
6	0	0	63	56
6	0	1*	0	26
6	0	2	112	108
6	0	3	54	57
6	0	4	86	85
6	0	5	162	172
6	0	6	77	69
6	0	7	73	72
6	1	0	104	104
6	1	2	114	118
6	1	4	38	41
6	1	5	40	35
6	1	6	81	79
6	1	7*	0	17
6	1	8	69	75
6	2	0	30	31
6	2	2	29	31
6	2	3	89	84
6	2	4	223	218
6	2	6*	0	2
6	2	7	129	135
6	2	8	61	65
6	3	0	170	183
6	3	2	178	192
6	3	4	76	67
6	3	5	138	130
6	3	7	74	73
6	3	8	140	127
6	3	9	45	44
6	4	0	210	226
6	4	4	34	31
6	4	5	61	63
8	3	0	56	53
8	3	2	70	66
8	3	3	80	79
8	3	5	32	28
8	3	6	57	52
8	3	7	33	26
8	3	8	38	42
8	3	9	53	54
8	4	-1*	0	10
8	4	0	97	100
8	4	4	50	53
8	4	5	55	57
8	4	6	60	58
8	4	7*	0	4
8	4	8	78	84
9	4	0*	0	17

mentioned in books and review articles (see *e.g.* Wells, 1962, p. 587). By contrast, West (1934) pointed out the chains of face-shared octahedra of composition $Li(OH_2)_3$ in $Li(ClO_4).3H_2O$, and these chains are mentioned in texts and review articles (see Wells, 1962, p. 583). This shows the importance of adequate descriptions of geometric and topologic features of crystal structures. Such descriptions are an aid in visualizing and classifying crystal structures.

The coordination octahedra around both Mg atoms can be formulated as $[MgO_2(OH_2)_4]^{2+}$, with the sulfate oxygen atoms in *trans* positions. Thus, they differ from the $[MgO_2(OH_2)_4]^{2+}$ octahedra in $MgSO_4.4H_2O$ (Baur, 1962) where the sulfate oxygen atoms were found in *cis* positions. The mean value of 2·063 Å for the bond distance Mg–O compares well with the corresponding distance of 2·065 Å in $MgSO_4.7H_2O$ (Baur, 1964). Both octahedra are slightly, but significantly, distorted in such a way that the distance to the sulfate oxygen atoms is the longest. For the case of Mg(2)–O(2) [0·045 Å longer than Mg(2)–O(*W*7,*W*8)], this could be rationalized on the basis of the extended electrostatic valence rule (Baur, 1970), since O(2) is the oxygen atom receiving the highest bond strength of all oxygen atoms (see Table 6). This explanation is not possible for Mg(1)–O(1) [0·037 Å longer than Mg(1)–O(*W*5,*W*6)], because in the Mg(1) octahedron all oxygen atoms receive the same bond strength. Since the longer Mg bonds to O(1) and O(2) in $MgSO_4.5H_2O$ correspond to the very long bonds, Cu–O in $CuSO_4.5H_2O$, it is conceivable that this lengthening is caused by a structural control. The relationship between bond strength and bond length is better displayed by the sulfate group, where the distances [Table 5(*a*)] vary exactly as the bond strengths (Table 6). This is not surprising, because an analysis of the bond-strength bond-length correlations for 14 different coordinations (Baur, 1970) has shown that the correlation coefficient is the higher, the larger the formal valence of the central cation in question There fore, we should expect a better agreement for the S^{6+}–O bonds than for the Mg^{2+}–O bonds.

The hydrogen bonds in $MgSO_4.5H_2O$ are arranged as in $CuSO_4.5H_2O$ [Table 5(*c*)]. The proposed hydrogen bonding scheme is substantiated by; (1) the analogy with $CuSO_4.5H_2O$, analyzed by neutron diffraction (Bacon & Curry, 1962); (2) the X-ray diffraction

Table 3. $MgSO_4.5H_2O$, *positional parameters in fractional coordinates and thermal parameters (both* $\times 10^4$*) with their standard deviations*

The definition of the Debye–Waller temperature factor is $\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)]$; the equivalent isotropic temperature factor B is (Hamilton, 1959):

$$\tfrac{4}{3}(\beta_{11}a^2+\beta_{22}b^2+\beta_{33}c^2+2\beta_{12}ab\cos\gamma+2\beta_{13}ac\cos\beta+2\beta_{23}bc\cos\alpha).$$

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B(Å²)
Mg(1)	0000	0000	0000	93 (4)	18 (1)	78 (3)	−5 (2)	−22 (3)	−2 (1)	1·0 (1)
Mg(2)	5000	5000	0000	68 (3)	18 (1)	61 (3)	6 (2)	22 (2)	−2 (1)	0·8 (1)
S	0371 (1)	2897 (1)	6624 (1)	60 (2)	17 (1)	53 (2)	3 (1)	12 (1)	0 (1)	0·8 (1)
O(1)	9464 (4)	1509 (2)	7309 (3)	125 (6)	23 (2)	104 (5)	−10 (3)	14 (4)	15 (2)	1·5 (2)
O(2)	2680 (4)	3344 (2)	8331 (3)	83 (5)	28 (2)	128 (5)	−2 (3)	−19 (4)	−14 (2)	1·5 (2)
O(3)	8808 (4)	3711 (2)	6610 (3)	126 (6)	46 (2)	128 (5)	44 (3)	36 (4)	−8 (2)	1·6 (2)
O(4)	0590 (4)	2986 (2)	4256 (3)	135 (6)	38 (2)	74 (4)	−12 (3)	−56 (4)	−3 (2)	1·4 (2)
O(*W*5)	8279 (4)	0768 (3)	1639 (4)	192 (8)	39 (2)	186 (6)	−4 (4)	114 (5)	−32 (3)	2·0 (2)
O(*W*6)	3086 (4)	1139 (3)	1848 (4)	149 (7)	32 (2)	119 (5)	−8 (3)	12 (4)	−6 (2)	1·8 (2)
O(*W*7)	4745 (4)	4042 (3)	3153 (4)	118 (6)	52 (3)	85 (5)	13 (3)	28 (4)	16 (2)	1·7 (2)
O(*W*8)	7567 (4)	4077 (3)	0318 (4)	116 (6)	63 (3)	104 (5)	47 (3)	22 (4)	−6 (3)	1·7 (2)
O(*W*9)	4589 (4)	1324 (3)	6699 (4)	113 (7)	51 (3)	178 (6)	9 (3)	35 (5)	6 (3)	2·1 (2)

Table 4. $MgSO_4.5H_2O$ *and* $MgCrO_4.5H_2O$, *coordinates of the hydrogen atoms* ($\times 10^3$) *as deduced from least-squares refinement* (LS), *difference synthesis* (Diff), *calculation of least electrostatic energy* (El), *and geometrical calculations based on the assumed hydrogen bonding arrangement* (Geom)

	$MgSO_4.5H_2O$													$MgCrO_4.5H_2O$		
	LS			Diff			El			Geom			Geom		
	x	y	z	x	y	z	x	y	z	x	y	z	x	y	z
H(54)	908 (15)	146 (8)	260 (13)	910	140	250	892	151	262	911	155	250	899	147	248
H(59)	724 (14)	023 (8)	230 (13)	730	020	220	703	017	212	737	016	253	733	010	247
H(62)	331 (13)	192 (7)	117 (12)	330	200	140	365	201	118	325	209	148	323	213	116
H(69)	336 (12)	148 (8)	321 (11)	330	140	350	377	110	355	354	095	355	353	112	335
H(73)	562 (13)	402 (8)	411 (11)	580	380	430	615	394	441	603	386	450	582	388	439
H(74)	350 (15)	392 (8)	349 (10)	360	380	380	344	375	376	331	368	352	316	367	331
H(83)	786 (13)	385 (9)	919 (14)	790	400	920	816	394	911	804	394	902	811	396	908
H(84)	842 (13)	374 (8)	179 (12)	850	400	160	862	389	187	852	373	179	854	377	179
H(91)	585 (13)	115 (8)	733 (11)	610	120	740	625	167	715	621	141	692	622	130	673
H(92)	433 (13)	201 (9)	706 (10)	420	200	720	385	196	698	440	206	734	458	206	721

evidence (see Table 4); (3) the calculation results of the positions of least electrostatic energy of the hydrogen atoms (Table 4) [the charges assumed on the different atoms were: magnesium, +2·0 e; sulfur, 0·0 e; sulfate oxygen, −0·5 e; water oxygen −1·0 e; hydrogen, +0·5 e. The shape of the water molecule was held constant (angle H–O(*W*)–H = 109·5°, O(*W*)–H = 0·97 Å). The computation was performed in the same way as for $CuSO_4.5H_2O$ (Baur, 1965)]; (4) a consideration of the interatomic distances and angles between the O(*W*) atoms and the surrounding magnesium and oxygen atoms (see the following paper, Baur, 1972). The results of this geometrical calculation for $MgSO_4.5H_2O$ and $MgCrO_4.5H_2O$ (Bertrand, Dusausoy, Protas & Watelle-Marion, 1971) are given in Table 4.

The distances and angles involving hydrogen atoms [Table 5(*c*)] are based, for $MgSO_4.5H_2O$, on the electrostatically calculated hydrogen atom positions, for $MgCrO_4.5H_2O$ on the geometrical calculation, and for $CuSO_4.5H_2O$ on the neutron diffraction results. The errors of the distances and angles involving hydrogen atoms for $CuSO_4.5H_2O$ are ±0·01 Å and ±1·0° respectively. It is assumed that the positions calculated for the hydrogen atoms in $MgSO_4.5H_2O$ are on the average within 0·1 Å of the positions as they could be determined by neutron diffraction, while for $MgCrO_4.5H_2O$ this estimated error margin is 0·2 Å (see Baur, 1972). The hydrogen bonding geometry [Table 5(*c*)] is very similar for the three salts. Larger discrepancies occur for the H···O(1) and H···O(2) distances, in which O(*W*9) is the donor. These are the bonds which have the most pronounced differences in the O(*W*) → O distances between the three compounds. They seem to be due to the different shape of the Cu-coordination octahedron as compared to the Mg octahedra. The Cu(1)–O(1) and Cu(2)–O(2) distances are much longer than the Cu–O(*W*) distances; therefore, the tetrahedron is displaced in the Cu salt relative to its position in the Mg salts, in which the Mg octahedra are more regular. Similarly, the hydrogen bonds are affected by the larger size of the chromate group as compared with the sulfate group. Therefore, the position of the O(*W*9) atom and the lengths of its bonds are different in the three salts.

The mean length of all hydrogen bonds is 0·05 Å longer in the Mg salts than in the Cu salt [Table (5*c*)]. The shorter mean hydrogen bond length in the Cu salt is mainly due to the shortness of those O(*W*) → O bonds which originate at the water molecules bonded into the square-planar coordination around the Cu ions. The same effect can be observed in the only other pair of isostructural hydrated Cu and Mg salts of which the crystal structures have been determined: $Mg(NH_4)_2(SO_4)_2.6H_2O$ (Margulis & Templeton, 1962) and $Cu(NH_4)_2(SO_4)_2.6H_2O$ (Brown & Chidambaram, 1969). In these salts, the hydrogen bonds donated by the water molecules bonded in the square-planar

Table 5. *Interatomic distances and bond angles in* $MgSO_4.5H_2O$, $MgCrO_4.H_2O$ (*Bertrand et al.*, 1971) *and* $CuSO_4.5H_2O$ (*Bacon & Curry*, 1962)

The e.s.d.'s involving nonhydrogen atoms are equal to or smaller than ±0·005, ±0·02 and ±0·02 Å respectively for the bond lengths, and equal to or smaller than ±0·2, ±0·7 and ±1·0° respectively for the bond angles.
For distances and angles involving hydrogen atoms see text.

	Mg,S salt	Mg,Cr salt	Cu,S salt
(*a*) Tetrahedral group			
T–O(1)	1·471 Å	1·64 Å	1·48
T–O(2)	1·477	1·65	1·49
T–O(3)	1·462	1·62	1·47
T–O(4)	1·467	1·64	1·50
Mean of 4	1·469	1·636	1·484
Range of 6 O–O	2·39–2·42	2·65–2·70	2·41–2·44
Mean of 6 O–O	2·399	2·671	2·423
Range of 6 O–T–O	108·2–110·8°	108·7–111·4°	108·3–111·0°
Mean of 6 O–T–O	109·5	109·5	109·5
(*b*) Octahedral groups			
2 × M(1)–O(*W*6)	2·049 Å	2·08 Å	1·98 Å
2 × M(1)–O(*W*5)	2·059	2·03	1·99
2 × M(1)–O(1)	2·091	2·08	2·38
2 × M(2)–O(*W*8)	2·038	2·06	1·95
2 × M(2)–O(*W*7)	2·046	2·04	1·98
2 × M(2)–O(2)	2·097	2·08	2·43
Mean of 12	2·063	2·063	2·118
Mean of 8 short Cu–O(*W*) bonds			1·974
Mean of 4 long Cu–O bonds			2·407
Range of 24 O–O	2·844–3·002	2·88–2·97	2·77–3·19
Mean of 24 O–O	2·918	2·918	3·005
Range of 24 O–M–O	86·9–93·1°	88·6–91·4°	87·0–93·0°

Table 5 (*cont.*)

(*c*) Water molecules

	Mg,S salt	Mg,Cr salt	Cu,S salt
O(*W*5)→O(4)	2·802 Å	2·78 Å	2·83 Å
O(*W*5)→O(*W*9)	2·755	2·84	2·76
H(54)–O(4)	1·84	1·81	1·91
H(54)–O(*W*9)	1·83	1·89	1·81
O(4)–O(*W*5)–O(*W*9)	120·8°	122·0°	120·5°
O(*W*5)–H(54)–O(4)	169	175	168
O(*W*5)–H(59)–O(*W*9)	160	166	171
O(*W*6)→O(2)	2·890 Å	2·91 Å	2·80 Å
O(*W*6)→O(*W*9)	2·773	2·81	2·75
H(62)–O(2)	2·07	2·07	1·90
H(69)–O(*W*9)	1·82	1·85	1·76
O(2)–O(*W*6)–O(*W*9)	125·4°	126·3°	130·0°
O(*W*6)–H(62)–O(2)	142	144	154
O(*W*6)–H(69)–O(*W*9)	165	168	171
O(*W*7)→O(3)	2·768 Å	2·75 Å	2·70 Å
O(*W*7)→O(4)	2·828	2·77	2·75
H(73)–O(3)	1·80	1·80	1·73
H(74)–O(4)	1·88	1·80	1·79
O(3)–O(*W*7)–O(4)	117·1°	119·4°	118·7°
O(*W*7)–H(73)–O(3)	177	165	176
O(*W*7)–H(74)–O(4)	167	180	168
O(*W*8)→O(3)	2·715 Å	2·73 Å	2·68 Å
O(*W*8)→O(4)	2·796	2·70	2·72
H(83)–O(3)	1·75	1·77	1·72
H(84)–O(4)	1·87	1·76	1·79
O(3)–O(*W*8)–O(4)	104·3°	105·5°	105·2°
O(*W*8)–H(83)–O(3)	171	169	173
O(*W*8)–H(84)–O(4)	158	163	167
O(*W*9)→O(1)	2·931 Å	2·82 Å	2·79 Å
O(*W*9)→O(2)	3·115	3·23	3·00
H(91)–O(1)	2·05	1·85	1·84
H(92)–O(2)	2·16	2·32	2·07
O(1)–O(*W*9)–O(2)	125·5°	123·2°	122·1°
O(*W*9)–H(91)–O(1)	150	174	167
O(*W*9)–H(92)–O(2)	168	156	161
Mean of all 10 H bonds	2·837	2·83	2·78
Mean of 8 bonds donated by O(*W*5), O(*W*6), O(*W*7), O(*W*8)	2·791	2·79	2·75
Mean of 2 bonds accepted by O(2), $\Delta p = -0{\cdot}17$ v.u.	3·003	3·07	2·90
Mean of 2 bonds accepted by O(3), $\Delta p = 0{\cdot}17$ v.u.	2·742	2·74	2·69
Mean of 6 bonds accepted by O(1), O(4), O(*W*9), $\Delta p = 0$	2·814	2·79	2·77

coordination have a mean length of 2·716 Å, while the corresponding bonds in the Mg salt have a mean length of 2·742 Å. Water molecules bonded into the square-planar coordination around a Cu atom seem to form stronger hydrogen bonds than water molecules bonded to Mg atoms.

The mean bond length of a hydrogen bond between oxygen atoms can be predicted with a mean deviation of 0·08 Å from the empirical relation (Baur, 1970, 1972):

$$d(\text{O–H}\cdots\text{O}) = (2{\cdot}85 - 0{\cdot}38\Delta p)\ \text{Å}\,,$$

where Δp is the difference between the values of p_{O} received by the donor atom and the acceptor atom of the hydrogen bond. The predicted hydrogen bond lengths for $\text{MgSO}_4.5\text{H}_2\text{O}$ are compared with the observed values in Table 7. The same formalism can be applied to the hydrogen bonds in $\text{CuSO}_4.5\text{H}_2\text{O}$. Since the differences in Cu–O bond length within the distorted coordination octahedra around Cu^{2+} are not due to Δp_{O} variations, but are due instead to an inherent asymmetry of the Cu^{2+} ions, it appears to be reasonable to assign different bond strengths to the short (0·4v.u.) and the long (0·2v.u.) Cu–O bonds (Table 6). Therefore, the average Δp for the hydrogen bonds in the Cu salt is +0·10v.u., as compared with 0·0v.u. for the Mg salts. The individual and the mean deviations of observed and calculated hydrogen bond lengths (Table 7) are within the range of values found in the much larger sample of 392 hydrogen bonds investigated previously (Baur, 1970).

Crystal symmetry of Cu salts

The detailed geometry of the chains of octahedra and tetrahedra is different in the three salts, because of the slightly differing dimensions of the octahedral and tetrahedral groups. For one, these differences are reflected in the unit-cell parameters. Secondly, the chains of octahedra and tetrahedra connected by the bonds -M(1)-O(1)-T-O(2)-M(2)- are more kinked in $CuSO_4.5H_2O$ and $MgCrO_4.5H_2O$ than in $MgSO_4.5H_2O$. The centroids of the tetrahedral groups are displaced by about 0·25 Å in the Cu salt, and by about 0·15 Å in the chromate, away from the line M(1)-M(2) as compared with $MgSO_4.5H_2O$. Such changes are possible, because the hydrogen bonds that connect the chains are weak compared with the M-O and T-O bonds and are able to adjust themselves to the changes. It appears that this ability of a crystal structure type to absorb changes in the size and distortion of the MO_6 coordination polyhedron is a necessary condition for the occurrence of strictly isostructural Mg and Cu salts. However, it is clearly not a sufficient condition, otherwise there should be more examples of strictly isostructural pairs, especially among highly hydrated salts. No additional explanation for the occurrence or absence of isostructural pairs of Cu and Mg salts can be offered here; however, it should be pointed out that the question is too complex to be solved simply by a reference to the static Jahn–Teller effect. Occasionally, the opinion is voiced that the lowering of the symmetry of a Cu compound, as compared with the analogous Mg compound (or other compounds with first-row transition elements), is due to the distortion of the Cu coordination by the Jahn–Teller effect. For example, monoclinic CuF_2 crystallizes in a distorted rutile type (Billy & Haendler, 1957), while the difluorides of Mg, Mn, Fe, Co, Ni, and Zn (Baur, 1958) represent the undistorted tetragonal rutile type. According to Creighton (1971), this is a most convincing example of a distortion caused by the Jahn–Teller effect, because in the tetragonal rutile compounds there is 'an almost perfect regular octahedral arrangement', while in CuF_2 the coordination is tetragonal with four short and two long bonds. Actually, however, the local symmetry around the cations is orthorhombic (*mmm*) even in the tetragonal rutile-type crystals, and this ortho-

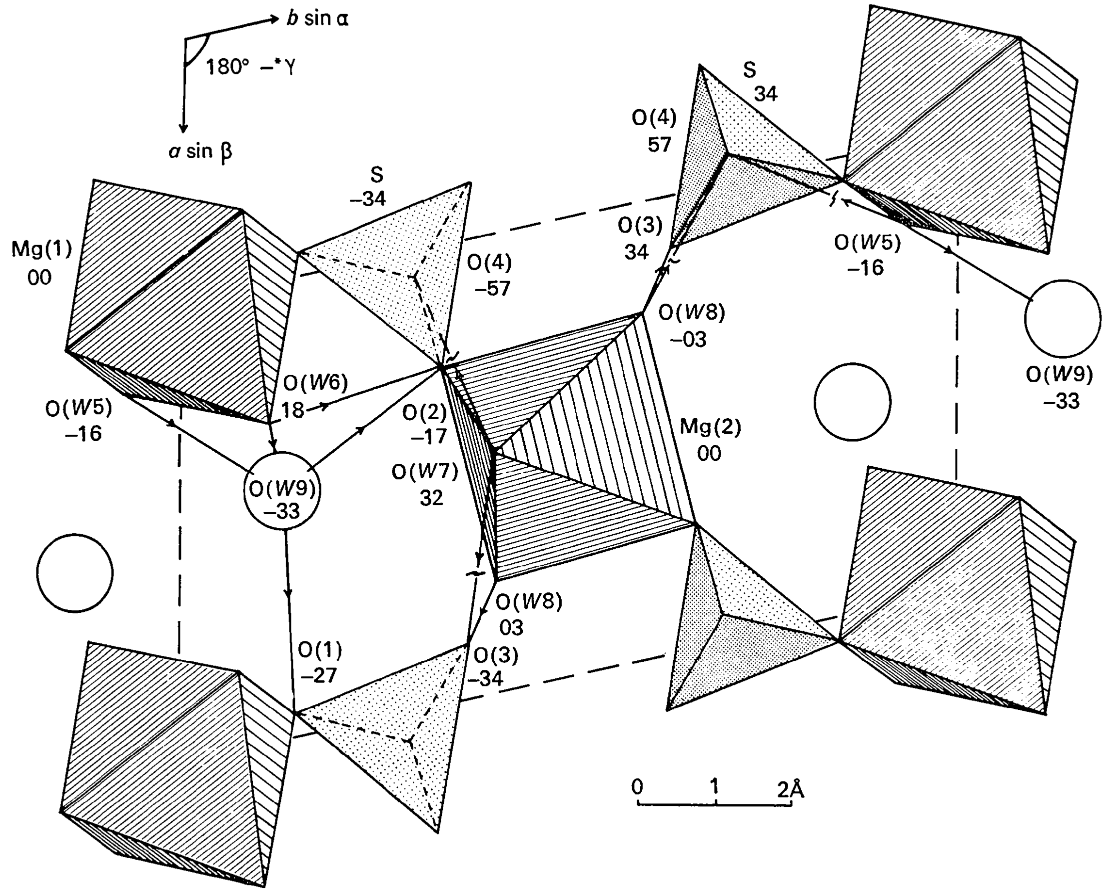

Fig. 1. $MgSO_4.5H_2O$, view parallel to [001]. Polyhedral representation, except for the O(*W*9) atoms, which are shown as circles. Some of the hydrogen bonds are indicated as arrows pointing from the donor to the acceptor atoms. The complete hydrogen bonding environment of every oxygen atom is displayed once. The heights of some of the central atoms of the polyhedra and of selected oxygen atoms are indicated in fractional coordinates × 100.

Table 6. $MgSO_4.5H_2O$ *and* $CuSO_4.5H_2O$, *electrostatic bond strengths* (*Pauling*, 1960, *p*. 547; *Baur*, 1970)

The hydrogen atom contribution to the hydrogen bond donor is identified as H(*d*), to the acceptor as H(*a*).

⁄	Mg salt						Cu salt		
	Mg(1)	Mg(2)	S	H(*a*)	H(*d*)	p_O	Cu(1)	Cu(2)	p_O
O(1)	$\frac{1}{3}$		$\frac{6}{4}$	$\frac{1}{6}$		2·00 v.u.	$\frac{2}{10}$		1·87 v.u.
O(2)		$\frac{1}{3}$	$\frac{6}{4}$	$2\times\frac{1}{6}$		2·17		$\frac{2}{10}$	2·04
O(3)			$\frac{6}{4}$	$2\times\frac{1}{6}$		1·83			1·83
O(4)			$\frac{6}{4}$	$3\times\frac{1}{6}$		2·00			2·00
O(*W*5)	$\frac{1}{3}$				$2\times\frac{5}{6}$	2·00	$\frac{4}{10}$		2·07
O(*W*6)	$\frac{1}{3}$				$2\times\frac{5}{6}$	2·00	$\frac{4}{10}$		2·07
O(*W*7)		$\frac{1}{3}$			$2\times\frac{5}{6}$	2·00		$\frac{4}{10}$	2·07
O(*W*8)		$\frac{1}{3}$			$2\times\frac{5}{6}$	2·00		$\frac{4}{10}$	2·07
O(*W*9)				$2\times\frac{1}{6}$	$2\times\frac{5}{6}$	2·00			2·00

Table 7. *Comparison of observed and calculated* [*equation* (1)] *hydrogen bond lengths in* $MgSO_4.5H_2O$ *and* $CuSO_4.5H_2O$

	$MgSO_4.5H_2O$				$CuSO_4.5H_2O$			
	Δp	d_{obs}	d_{calc}	$\vert\Delta\vert$	Δp	d_{obs}	d_{calc}	$\vert\Delta\vert$
O(*W*5)→O(4)	0·0 v.u.	2·80 Å	2·85 Å	0·05 Å	0·07 v.u.	2·83 Å	2·82 Å	0·01 Å
O(*W*5)→O(*W*9)	0·0	2·76	2·85	0·09	0·07	2·76	2·82	0·06
O(*W*6)→O(2)	−0·17	2·89	2·91	0·02	0·03	2·80	2·84	0·04
O(*W*6)→O(*W*9)	0·0	2·77	2·85	0·08	0·07	2·75	2·82	0·07
O(*W*7)→O(3)	0·17	2·77	2·79	0·02	0·24	2·70	2·76	0·06
O(*W*7)→O(4)	0·0	2·83	2·85	0·02	0·07	2·75	2·82	0·07
O(*W*8)→O(3)	0·17	2·72	2·79	0·07	0·24	2·68	2·76	0·08
O(*W*8)→O(4)	0·0	2·80	2·85	0·05	0·07	2·72	2·82	0·10
O(*W*9)→O(1)	0·0	2·93	2·85	0·08	0·13	2·79	2·80	0·01
O(*W*9)→O(2)	−0·17	3·12	2·91	0·21	−0·04	3·00	2·87	0·13
Mean	0·0			0·07	0·10			0·06

rhombic symmetry is very clearly displayed in all crystals (Baur & Khan, 1971). CuF_2 could crystallize in the undistorted rutile type and have a very distorted coordination octahedron, of the same type as in the monoclinic CuF_2 phase, since the lattice symmetry of a crystal does not have to coincide with a local site symmetry. The difference between CuF_2 and the undistorted rutile type may lie in the possibility of achieving a 2+2+2 coordination (with three different Cu–F bond lengths), or in a nonplanar coordination of Cu around F. Both these arrangements definitely are not allowable by the symmetry of the undistorted rutile type. In the crystal structure of CuF_2 as reported by Billy & Haendler (1957), there is no indication of these additional distortions. However, the structure has not been determined with sufficient accuracy to exclude them. The finding of such distortions could give a clue as to why CuF_2 crystallizes in a distorted rutile type. The presence of the Jahn–Teller effect, by itself, is not a sufficient explanation.

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