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Crystallographic properties of $CuSO_4 . H_2O$ and $ZnSO_4 . H_2O$.

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Cupric sulfate monohydrate was prepared by heating Merck reagent grade $CuSO_4 . 5\,H_2O$ to 120 °C for 3 hr. The company's analysis of the impurities present in the more hydrated material is as follows: Insoluble 0·005%, chloride (Cl) 0·0005%, nitrogen (N) 0·004%, nickel 0·002%, iron 0·005%, alkalies and earths 0·1%.

Zinc sulfate monohydrate was prepared by heating Merck reagent grade $ZnSO_4 . 7\,H_2O$ to 120 °C for one hr. The company's analysis is as follows: Insoluble 0·005%, Cl 0·0003%, nitrate (NO_3) 0·001%, iron 0·0001%, manganese 0·0003%, ammonia (NH_4) 0·002%, alkalies and earths 0·1%.

In both cases the weight loss after heating agreed with the expected values.

The X-ray powder diffraction patterns of the finely ground monohydrates at 25 °C were obtained in a Philips high-angle recording diffractometer, using filtered Co $K\alpha$ radiation ($\lambda = 1{\cdot}7902$ Å). The instrument was calibrated against high-purity silicon.

The assignment of the peaks was made by using the axial ratios of natural szomolnokite, which is monoclinic prismatic (Dana & Dana, 1951). All the observed diffraction peaks could be satisfactorily indexed as being due to a monoclinic lattice with the following unit-cell dimensions, obtained by least-squares:

	$CuSO_4 . H_2O$	$ZnSO_4 . H_2O$
a_0 =	7·635 ± 0·010 Å	7·566 ± 0·008 Å
b_0 =	7·426 ± 0·010	7·586 ± 0·008
c_0 =	7·176 ± 0·010	6·954 ± 0·008
β =	116° 9′ ± 2′	115° 56′
$a:b:c$ =	1·028:1:0·9664	0·9974:1:0·9167

Table 1. *Powder data for* $CuSO_4 . H_2O$ *and* $ZnSO_4 . H_2O$

	$CuSO_4 . H_2O$		
hkl	d_o	d_c	100 I/I_0
011	4·860 Å	4·866 Å	30
$11\bar{1}$	4·793	4·791	40
111	3·458	3·461	25
200	3·430	3·427	100
$21\bar{1}$	3·375	3·381	80
$20\bar{2}$	3·136	3·136	75
$12\bar{2}$	2·582	2·580	20
220	2·517	2·518	18
022	2·431	2·433	15
$11\bar{3}$	2·259	2·256	25
$21\bar{3}$	2·231	2·234	15
$13\bar{1}$	2·094	2·092	5
013	2·066	2·063	8
320	1·943	1·946	2
311	1·846	1·845	2
$41\bar{1}$	1·817	1·817	7
$20\bar{4}$, 140	1·793	1·793, 1·792	5
$13\bar{3}$, 400	1·712	1·711, 1·713	5
$23\bar{3}$	1·702	1·701	5
$42\bar{2}$	1·689	1·690	7
033	1·619	1·622	5
$33\bar{3}$, $24\bar{2}$	1·596	1·597, 1·597	15
$40\bar{4}$	1·568	1·568	6
$32\bar{4}$	1·562	1·561	6
142, $43\bar{1}$	1·492	1·494, 1·494	2
$51\bar{1}$	1·451	1·451	5

Table 1 (*cont.*)

	$ZnSO_4 . H_2O$		
hkl	d_o	d_c	100 I/I_0
011	4·824 Å	4·825 Å	40
$11\bar{1}$	4·772	4·768	53
020	3·799	3·793	15
200, 111	3·410	3·402, 3·428	100
$21\bar{1}$	3·356	3·366	23
120	3·313	3·313	27
$20\bar{2}$	3·063	3·065	45
$12\bar{2}$	2·561	2·563	15
220	2·525	2·532	38
211	2·420	2·422	3
022	2·411	2·413	4
$22\bar{2}$, $31\bar{1}$	2·386	2·384, 2·386	3
031	2·343	2·344	10
$13\bar{1}$	2·334	2·337	5
$11\bar{3}$	2·193	2·196	15
$21\bar{3}$	2·182	2·179	3
131	2·111	2·112	10
$23\bar{1}$	2·098	2·098	6
122	2·060	2·065	8
$31\bar{3}$	1·972	1·973	12
$40\bar{2}$	1·879	1·878	4
231	1·899	1·898	3
$42\bar{2}$	1·678	1·682	10
240	1·657	1·657	6
042	1·621	1·622	7
$33\bar{3}$	1·589	1·589	5
$32\bar{4}$, $40\bar{4}$	1·529	1·531, 1·532	2
142	1·502	1·502	5
213	1·478	1·479	4
051, $15\bar{1}$	1·473	1·474, 1·473	2
340	1·454	1·455	4
151	1·412	1·411	3
$24\bar{4}$, $52\bar{4}$, 431	1·281	1·281, 1·281, 1·280	5
{$15\bar{3}$, $14\bar{4}$, 440} {$25\bar{3}$, 060, 313}	1·262–1·266	{1·265, 1·263, 1·266} {1·262, 1·264, 1·263}	4 broad

The observed and calculated d-spacings, indices and relative intensities are listed in Table 1. The obvious selection rules are:

hkl: $k+l$ even.
$h0l$: all even.

The systematic absences (hkl absent if $k+l$ is odd; $h0l$ absent if either h or l is odd) indicate the space group C^6_{2h}–$A2/a$ or C^4_s–Aa. However, since kieserite, which is probably isostructural, belongs to the space group $A2/a$, this is also taken to be the space group in the present case.

The unit cells each contain four formula weights. This leads to a density at 25 °C of 3·231 g.cm.$^{-3}$ for $CuSO_4 . H_2O$ and of 3·321 g.cm.$^{-3}$ for $ZnSO_4 . H_2O$.

References

DANA, J. D. & DANA, E. S. (1951). *System of Mineralogy*, Vol. II. New York: John Wiley.