

the general position is $\pm(x, y, z; \bar{x}, \bar{y}, \frac{1}{2}+z; \bar{y}, x, \frac{3}{4}+z; y, \bar{x}, \frac{1}{4}+z)$ and let us find the phase relation corresponding to the symmetry operation $\mathbf{r}(xyz) \rightarrow \mathbf{r}'(\bar{y}, x, \frac{3}{4}+z)$.

This is done in four steps.

- (1) Form the scalar product
 $\mathbf{h} \cdot \mathbf{r}' = h(\bar{y}) + kx + l(\frac{3}{4}+z)$.
- (2) Isolate the translational component which gives rise to a phase factor $a = \exp 2\pi i \frac{3}{4}l = \exp(3\pi il/2)$.
- (3) Rewrite the resting scalar product in the form $\mathbf{r} \cdot \mathbf{h}' = xk + y(\bar{h}) + zl$, *i.e.* bring xyz into their usual sequence.
- (4) The desired symmetry relation between structure factors is
 $F(\mathbf{h}) = aF(\mathbf{h}')$, *i.e.*
 $F(hkl) = \exp(3\pi il/2)F(k\bar{h}l)$.

If the reader is able to show that to the points $\mathbf{r}(xyz)$ and $\mathbf{r}'(\frac{1}{4}-z, \frac{1}{4}-y, x)$ of group $Fd3m(O_h)$ No. 227 corresponds the phase relation $F(hkl) = F(\bar{k}\bar{h})\exp(\pi i(h+k)/2)$ he will probably have understood how to use the method.

The theoretical proof may be found in French (Bertaut, 1959), in English (Bertaut & Waser, 1957) and in German (Bertaut, 1958).

In Jeffery's (1963) notation, the phase relation under (4) reads

$$\alpha_{hkl} = \alpha_{k\bar{h}l} + (3\pi/2)l$$

whereas Jeffery writes

$$\alpha_{hkl} = \alpha_{\bar{k}hl} + (3\pi/2)l.$$

We must conclude and have checked that in Tables 1 and 2 given by Jeffery, $\alpha_{\bar{k}hl}$ should be replaced by $\alpha_{k\bar{h}l}$ and, *vice versa*, $\alpha_{k\bar{h}l}$ should be replaced by $\alpha_{\bar{k}hl}$.

Finally let us mention that all phase relations for centrosymmetric groups are given in *Tables de Linéarisation des Facteurs de Structure* (Bertaut & Dulac, 1955, 1956).

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Lattice constants of some double sulphates $M_2Co(SO_4)_2 \cdot 6H_2O$. By P. HARTMAN and C. F. WOENSDREGT, *Geologisch en Mineralogisch Instituut der Rijksuniversiteit, Garenmarkt 1b, Leiden, The Netherlands*

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The lattice constants of four isomorphous cobalt double sulphates $M_2Co(SO_4)_2 \cdot 6H_2O$, with $M = K, Rb, NH_4$ and Cs , have been determined from powder X-ray photographs with a quadruple Guinier—de Wolff camera (de Wolff, 1948) and $Cu K\alpha$ radiation. Because of the larger deviations on the two outer strips, only the inner ones were used, one recording the powder lines of the cobalt double sulphate, the other recording the lines of a reference substance for which we chose potassium aluminum alum. In a separate measurement on a Debye-Scherrer X-ray photograph taken in a cylindrical camera with 9 cm diameter the unit cell edge of the potassium aluminum alum was found to be 12.157_8 \AA , in excellent agreement with the value $12.158 \pm 0.001 \text{ \AA}$ found by Klug & Alexander (1940).

Calibration of each film was based on this value of the

alum unit cell edge. The measured line positions appeared to be, within the limits of errors, a linear function of the calculated positions.

Irregular deviations as found by Fisher (1957) were not observed.

With this linear function the line positions of the sulphates were corrected and the constants in the relation

$$\sin^2 \theta = Ah^2 + Bk^2 + Cl^2 + Dhl$$

were calculated. B was found from $\sin^2 \theta$ differences between hk_1l and hk_2l reflexions, A from $hk0$ reflexions, C from $0kl$ reflexions and from $\sin^2 \theta$ differences between hkl and $h\bar{k}l$ reflexions and D from all hkl reflexions. Table 1 gives the calculated lattice constants with the standard deviation of the mean. The morphological axial ratios were taken from Groth (1908).

Table 1. *Lattice constants of $M_2Co(SO_4)_2 \cdot 6H_2O$*

	K	Rb	NH_4	Cs
a_0	$9.061 \pm 0.003 \text{ \AA}$	$9.180 \pm 0.001 \text{ \AA}$	$9.247 \pm 0.001 \text{ \AA}$	$9.316 \pm 0.001 \text{ \AA}$
b_0	12.207 ± 0.001	12.433 ± 0.001	12.519 ± 0.001	12.824 ± 0.001
c_0	6.151 ± 0.002	6.230 ± 0.003	6.239 ± 0.001	6.365 ± 0.002
β	$104^\circ 48' \pm 2'$	$106^\circ 01' \pm 1'$	$107^\circ 02' \pm 1'$	$107^\circ 07' \pm 1'$
β (morph.)	$104^\circ 55'$	$106^\circ 01'$	$106^\circ 56'$	$107^\circ 08'$
Axial ratio	0.7423:1:0.5039	0.7384:1:0.5011	0.7386:1:0.4984	0.7265:1:0.4963
Axial ratio (morph.)	0.7404:1:0.5037	0.7391:1:0.5011	0.7392:1:0.4985	0.7270:1:0.4968

Table 2. Observed and calculated $10^5 \cdot \sin^2 \theta$ values of $M_2Co(SO_4)_2 \cdot 6H_2O$

M = K			M = Rb			M = NH ₄			M = Cs		
hkl	10 ⁵ · sin ² θ		hkl	10 ⁵ · sin ² θ		hkl	10 ⁵ · sin ² θ		hkl	10 ⁵ · sin ² θ	
	obs.	calc.		obs.	calc.		obs.	calc.		obs.	calc.
020	1601	1592	110	1144	1146	020	1518	1514	110	1110	1109
001	1694	1677	020	1544	1535	001	1670	1667	001	1602	1603
011	2074	2075	001	1661	1655	011	2048	2046	011	1963	1964
111	2266	2267	111	2189	2181	111	2148	2146	120	2192	2192
200	3096	3092	120	2300	2297	120	2276	2273	021	3048	3046
021	3271	3270	200	3046	3048	200	3033	3036	121	3154	3149
111	3420	3430	021	3192	3190	021	3182	3181	201	3305	3307
201	3598	3606	210	3435	3432	121	3282	3281	210	3363	{ 3355
211	4009	4004	130	4209	4216	201	3378	3385	111	3367	{ 3358
130	4348	4356	220	4580	4583	111	3470	3464	211	3667	{ 3667
121	4624	4625	131	5251	5251	211	3766	3764	130	3997	{ 3995
031	5261	5260	201	5935	5941	130	4170	4166	220	4435	{ 4437
131	5450	5451	040	6145	6140	220	4558	4550	121	4440	{ 4440
201	5937	5933	211	6325	6325	121	4600	4599	131	4954	{ 4953
211	6350	{ 6331	230	6508	6502	221	4895	4899	040	5771	{ 5772
040		{ 6370	140	6904	6902	031	5078	5074	201	5891	{ 5888
002	6711	{ 6711	311	7030	7038	131	5174	5174	112	6233	{ 6232
112		{ 6717	202	7184	7188	201	6020	6021	311	6771	{ 6764
310	7367	7355	310	7243	7241	040	6061	6056	012	6771	{ 6774
221	7511	7525	221	7466	7476	211	6399	6400	202	6821	{ 6826
212	7894	{ 7872	212	7572	7572	112	6491	{ 6488	310	7097	{ 7097
122		{ 7911	122	7681	7677	131		{ 6492	122	7322	{ 7314
141	8236	8238	041	7801	7795	140	6815	6815	221	7331	{ 7331
321	8487	8481	141	7929	7938	311	6899	6900	141	7485	{ 7479
231	9521	9516	321	8183	8189	202	7068	7069	321	7837	{ 7847
331	10468	10472	320	8397	8393	310	7211	7210	320	8181	{ 8180
241	12299	12303	222	8712	8723	221	7535	7537	240	8771	{ 8766
250	13060	{ 13044	240	9188	9188	122	7621	7624	141	8770	{ 8770
042		{ 13079	231	9388	9395	321	8033	8034	241	9103	{ 9079
242	13840	13844	132	9601	{ 9595	112	9120	9124	132	9103	{ 9118
420	13963	{ 13960	241		{ 9604	231	9429	9428	312		{ 9638
331		{ 13963	331	10113	10108	312	9929	{ 9925	331	{ 9650	
			051	11258	11249	331		{ 9928	032	{ 9661	
			411	11743	11752	122	10253	10260	122	9896	{ 9896
			321	11898	11905	241	12082	12078	330	9982	{ 9983
			132	12068	{ 12073	212	12726	{ 12719	051	10616	{ 10622
			241		{ 12082	042		{ 12725	311		{ 10637
			042	12774	{ 12759	340	12884	12887	322	10711	{ 10720
			341		{ 12794	420	13653	13658	151	10711	{ 10725
			251	13061	13058			411	11362		{ 11358
			242	13323	13329						
			420	13722	13726						
			203	14228	{ 14222						
			412		{ 14238						
			003	14881	14891						

Table 2 lists the observed $\sin^2 \theta$ values of the measured reflexions, together with the calculated values.

The crystals were prepared by Mrs. H. Zandbergen of the Kamerlingh Onnes Laboratorium and the X-ray photographs were taken by Mr. A. Verhoorn.

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Paramètres et groupes spatiaux du chlorodurène et du bromodurène. Par G. CHARBONNEAU, J. BAUDOUR, J. CL. MESSAGER et J. MEINNEL, *Groupe de Recherches de physicochimie structurale, Faculté des Sciences de Rennes, France*

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Les mesures diélectriques ont montré que de nombreux dérivés pentasubstitués du benzène présentaient du polymorphisme. Nous avons entrepris l'étude des struc-

tures de différentes phases du chloro-1-tétraméthyl-2,3,5,6-benzène (monochlorodurène) et du bromo-1-tétraméthyl-2,3,5,6-benzène (monobromodurène). Nous avons