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The Crystal Structure of Mn_2Hg_5*

By J. F. de Wet†

National Chemical Research Laboratory, South African Council for Scientific and Industrial Research, Pretoria, South Africa

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The crystal structure of Mn_2Hg_5, a phase present in manganese amalgam at room temperature, is tetragonal (probable space group $P4/mbm$) with two formula units in a cell of dimensions $a = 9{\cdot}758$, $c = 2{\cdot}998$ Å. As the phase crystallizes in microscopic needles which are susceptible to atmospheric oxidation, special techniques for growing, handling and mounting the crystals were developed. A tentative structure was derived from packing considerations and was refined by Fourier methods. The structure may be regarded as built up of alternating layers of mercury and manganese atoms parallel to the basal plane. Its most interesting features are its close resemblance to the structure of $Pd(NH_3)_4Cl_2.H_2O$ and the hitherto unobserved 'twinned icosahedral' co-ordination around the manganese atoms. It is shown that this type of co-ordination is not restricted to this phase alone, but also occurs in the phases Si_2U_3 and Al_2Th_3.

1. Introduction

The existence of the phase Mn_2Hg_5 has been reported by several investigators (Prelinger, 1893; Royce & Kahlenberg, 1931; Lihl, 1955; De Wet, 1955). The first two workers obtained the compound by expressing excess of mercury from manganese amalgams, but its exact composition remained in doubt as a result of the unreliability of this method of isolation. De Wet (1955) succeeded in synthesising the compound in the form of pure crystals, and chemical analyses of these crystals, together with a comparison of the experimental density with that calculated from cell dimensions, confirmed the composition to be Mn_2Hg_5. While a preliminary account of the structure has been published (De Wet, 1957), subsequent work has led to a refinement of the structure and to a better understanding of its more interesting features.

2. Experimental techniques

(i) *Preparation of single crystals*

The preparation of single crystals suitable for study by X-ray diffraction proved to be one of the major problems in this work. Mn_2Hg_5 decomposes peritectically to MnHg and mercury at about 74 °C. (De Wet, 1955; Lihl, 1955), so that cooling of the melt results in the formation of a mass of small crystals, less than 1μ thick, rather than a few larger crystals. Methods for inducing the formation of somewhat larger crystals were then considered, since the optimum thickness (7μ for Cu $K\alpha$ radiation) indicated that quite small crystals could be used. Suitable crystals were obtained by heating a mixture of Mn_2Hg_5 and mercury, prepared by electrolysis of a manganese solution with a mercury cathode, until the compound had decomposed; the mixture was then maintained under vacuum for 12 weeks at 1–2° below the peritectic temperature in order to retard the rate of re-formation of Mn_2Hg_5. The crystals were finally isolated by centrifugation. The distinctly fibrous crystal habit, as well as a strong tendency for the needles to undergo basal cleavage, resulted in the occurrence of few usable crystals. The best specimens were found in the size range 0·2 to 0·3 mm. long and 5–15μ thick. Crystals prepared by the above technique were, however, susceptible to oxidation as a result of an adherent film of mercury, and tended to decompose in the atmosphere within a few days. Selected crystals were therefore mounted with the aid of a micro-manipulator and sealed off under argon in thin-walled Lindemann glass capillaries, in which they could be stored for mounting on a suitable single-crystal camera.

3. Crystallographic data

Oscillation photographs, taken about the needle axis at 90° intervals, established the tetragonal symmetry of the crystals. The a-spacing was determined with a Weissenberg camera, modified for back-reflection work according to Herbstein (1957). Four high-angle spots, with Bragg angles between 62·40 and 82·85°, were measured, and a weighted least-squares extrapolation of a against $\cos^2\theta$ gave the value $a = 9{\cdot}7577 \pm 0{\cdot}0018$ Å. As a similar procedure for determining c was not practicable, it was obtained by measuring accurately the 002 Bragg angle from a diffractometer trace; the instrument was calibrated with two neighbouring reflexions, 710 and 630, using the value of a given above. This led to value of $c = 2{\cdot}998 \pm 0{\cdot}0005$ Å and $c/a = 0{\cdot}3072$.

The density, determined by displacement as 12·85

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† Now at Physical Chemistry Department, University of Pretoria, Pretoria, South Africa.

g.cm.$^{-3}$, is in good agreement with the calculated value, assuming two formula units per cell, of 13·00 g.cm.$^{-3}$.

Using the multiple-film technique, intensities of the *hk*0 reflexions were measured visually against a standard scale of spots. Exposures were made on a Weissenberg camera, using Cu $K\alpha$ radiation; for determining the space-group conditions, equi-inclination photographs were taken of the *hk*1 and *hk*2 zones as well.

The only systematic absences observed were 0*kl* with *k* odd; these are consistent with any of the three space groups $P4/mbm$–D^5_{4h}, $P\bar{4}b2$–D^7_{2d} and $P4bm$—C^2_{4v}, of which only the first is centrosymmetric. Application of the statistical method (Howells, Phillips & Rogers, 1950) for detecting centrosymmetry was not considered very useful, since there would be too few atoms in general positions to ensure sufficient statistical randomness. A reasonable structure could, however, be derived on making the assumption that the manganese and mercury atoms lie on separate planes, namely $z=\frac{1}{2}$ and 0, respectively. This allocation of point positions is only compatible with the space group $P4/mbm$. The possibility of small deviations from these special values of the z-parameters, and therefore of one of the other two space groups, could not be entirely eliminated [see 4(ii)]; a study of the intensity trends between the even (*hk*0 and *hk*2) and odd (*hk*1) zones indicated, however, that deviations from the assumed structure are bound to be small. This does not affect the main points of discussion below, and, in what follows the two types of atom will be assumed to lie on interleaving planes spaced $c/2$ apart.

4. Determination of the structure

(i) *Derivation of a tentative structure*

A tentative structure could be derived from packing considerations, without any *a priori* assumption of the correctness of any of the above three space groups.

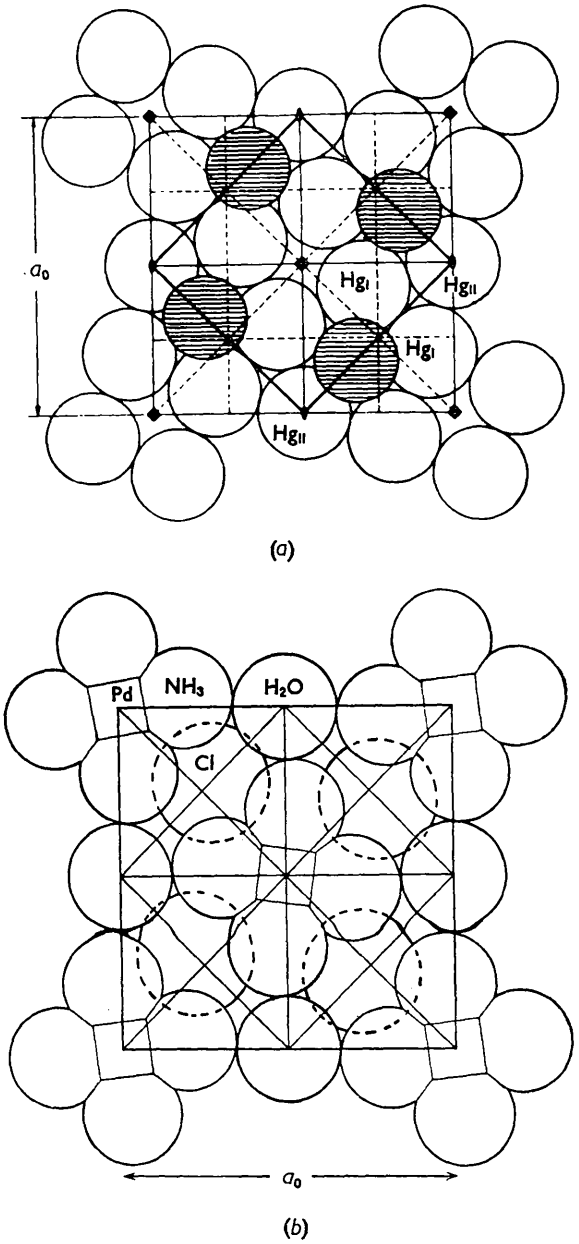

Fig. 1. (*a*) The unit cell of Mn_2Hg_5 (idealized model), viewed along the c-axis. (*b*) Projection of the structure of tetramminopalladium(II) chloride monohydrate on the plane (001). (After Dickinson, 1934).

The unusually small value of c, and its coincidence with the normal mercury diameter (3·00 Å) was suggestive of a planar, or nearly planar, arrangement of mercury atoms. The most probable distribution of the 10 atoms would be among one of the sets of 8-fold positions with x, y co-ordinates

$$\pm(x, y;\ y, x;\ x+\tfrac{1}{2}, \tfrac{1}{2}-y;\ y+\tfrac{1}{2}, x+\tfrac{1}{2})\ ,$$

which are common to the three space groups, and a 2-fold set of special positions. Now the 8-fold equipoint may be regarded as subdivided into two sets of four positions in square array, each around a 4-fold axis and reflected across the mirror planes parallel to (110). If eight mercury atoms are placed in these positions so that they are contiguous within a square group, and the square groups contiguous on the mirror planes, all can be accommodated in one plane, and sufficient room is left for two further mercury atoms at $(\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0)$—see Fig. 1. On stacking such planes directly above each other, the four manganese atoms can all be accommodated at a level exactly half-way between the mercury planes, if the manganese diameter is taken as 2·74 Å. This arrangement is only compatible with the following point positions (or their equivalents, translated along c by $\frac{1}{2}$) in $P4/mbm$:

8 Hg_I	in	8(*i*):	$(x, y, 0)$, etc.;
2 Hg_{II}	in	2(*d*):	$(\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0)$;
4 Mn	in	4(*h*):	$(x, x+\frac{1}{2}, \frac{1}{2})$, etc.

The relatively close-packed arrangement permitted the geometrical derivation of preliminary atomic parameters (Table 1) which gave a reasonable R-factor* of 35·2%.

(ii) *Refinement of the preliminary atomic parameters*

The small value of c and the absence of variable z-parameters permitted the refinement by Fourier projections down the c-axis only. After correcting the $hk0$ intensities for Lorentz and polarization factors, absorption and $\alpha_1-\alpha_2$ resolution in the usual way, the F_o values were brought to an absolute scale and an overall Debye–Waller temperature factor derived by plotting $\ln(F_c/F_o)$ against $\sin^2\theta/\lambda^2$. The atomic scattering factors used for F_c (Viervoll & Øgrim, 1949) were corrected for anomalous dispersion (Dauben & Templeton, 1955).

Table 1. *Atomic parameters*

	Geometrically derived		Final		
	x	y	x	y	$\sigma(x_n)$*
Hg_I	0·075	0·206	0·063	0·204	0·0008 (0·008 Å)
Mn	0·178	—	0·180	—	0·0025 (0·025 Å)

* Estimated by the method of Booth & Britten (1948).

Table 2. *Observed and calculated structure factors*

$hk0$	F_o	F_c	$hk0$	F_o	F_c
200	50	52	530	80	68
400	182	187	630	200	211
600	< 28	36	730	< 28	−18
800	155	−185	830	67	−85
10,00	65	76	930	< 28	20
110	< 14	9	440	96	95
210	63	−70	540	149	132
310	208	−240	640	< 28	23
410	341	−345	740	164	137
510	47	42	840	< 28	18
610	< 28	−30	940	156	−134
710	202	−239			
810	< 28	−22	550	206	−213
910	< 28	−21	650	106	101
10,10	57	50	750	149	−128
11,10	38	−55	850	85	−79
			950	180	−131
220	141	−144	10,50	< 28	38
320	208	−214	11,50	82	−71
420	180	170			
520	59	−52	660	51	60
620	186	174	760	< 28	−20
720	< 28	−17	860	53	56
820	125	127	960	< 28	−14
920	< 28	−29	10,60	< 28	−18
10,20	163	162	11,60	82	102
11,20	82	100			
			770	145	112
330	294	−297			
430	< 22	−27	880	200	158

Two Fourier refinement stages and a difference synthesis were carried out; the parameter refinements dictated by the F_o-F_c synthesis were less than the standard deviations of the atomic positions due to random errors of measurement (Table 1), and therefore no further refinement was undertaken. The geometrically derived parameters, as well as the final parameters, are given in Table 1; the observed structure amplitudes and structure factors calculated from the final parameters are compared in Table 2. The R-factor decreased, during refinement, from 35·0 to 10·4%, while the only significant parameter change was that in $x(Hg_I)$ from 0·075 to 0·063. The relatively poor quality of the crystals obtainable imposed limitations on the accuracy of the intensity data, so that further refinement, e.g. three-dimensional, or by making use of anisotropic or even separate atomic temperature factors, was not considered to be practicable. Accordingly, a final decision as to whether the mercury atoms are co-planar or slightly puckered, and therefore a rigorous proof of the correctness of the space group assignment, is not possible. The final value of the R-factor does, however, indicate that the chosen parameters cannot be greatly in error.

5. Interatomic distances

The standard deviation of the manganese atomic position is relatively large; although required by symmetry to lie on the (110) mirror plane, there is still a region of 0·2 Å within which this atom may be situated. Two locations within this region, namely (1) and (2) (Fig. 2), separated by 0·11 Å, confer the most symmetrical co-ordination on the manganese atom (the mercury atoms being regarded as fixed). In position (1), the manganese atom is equidistant from 8 mercury atoms (B, C, D, E and the ones above them); in position (2), the co-ordination is the same as that in

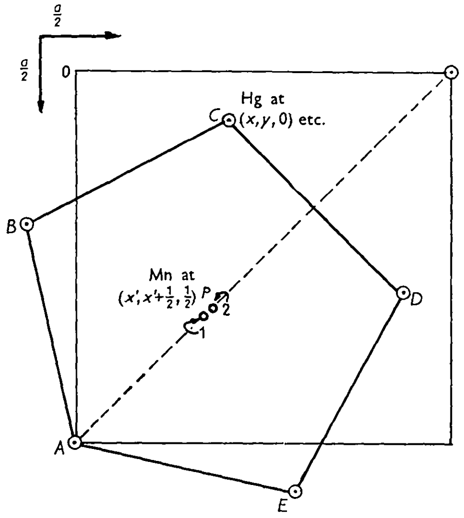

Fig. 2. Co-ordination of mercury atoms around a manganese atom in Mn_2Hg_5.

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* Absent reflexions were not included in this, and subsequent, R factors.

the idealized model [Fig. 1(*a*)], i.e., the manganese atom is equidistant from 6 mercury atoms (*A*, *C*, *D* and the ones above them), and equidistant, but further removed, from the remaining four. The calculated interatomic distances for these alternative locations, as well as those for the idealized structure, are given in Table 3, together with the distances calculated from the refined atomic positions. Although the differences in bond lengths are not, strictly speaking, significant, the bond lengths from the refined parameters are in better agreement with those corresponding to location (2), implying that the co-ordination symmetry around the manganese atom has not been altered by refinement.

The standard deviations of the Mn–Hg and Hg–Hg bond lengths, as estimated from the precision of the terminal atomic positions, are not considered to exceed 0·045 and 0·01 Å, respectively. It is certain, therefore, that the bond *C–D* is appreciably longer than the remaining Hg–Hg bonds. Although the mercury atoms *A–E* are no longer situated on the vertices of an equilateral pentagon, it is significant that the manganese atom is more nearly equidistant from its 12 neighbours than in the idealized model (Tables 3 and 4).

Table 3. *Comparison of experimental interatomic distances with those for various geometrical variants of the structure*

Bond	Idealized model	Mn in (1*)	Mn in (2*)	Experimental values
Mn–Hg (*PA**)	2·87 Å	2·83 Å	2·92 Å	2·90 Å
Mn–Hg (*PB, PE*)	3·10	3·00	3·02	3·02
Mn–Hg (*PC, PD*)	2·87	2·99	2·92	2·94
Mn–Mn	3·00	3·00	3·00	3·00
Hg–Hg (*AB, AE*)	3·00	—	—	2·95
Hg–Hg (*BC, DE*)	3·00	—	—	2·95
Hg–Hg (*CD*)	3·00	—	—	3·22

* See Fig. 2.

Table 4. *Nearest-neighbour distances in* Mn_2Hg_5
[Mn in position (2)*]

Central atom	Number of neighbours	Type of neighbour	Distance	Mean distance
Mn	4	Hg_I	2·92 Å	2·97 Å
	4	Hg_I	3·02	
	2	Hg_{II}	2·92	
	2	Mn	3·00	
Hg_I	2	Hg_I	2·95 Å	3·00 Å
	2	Hg_I	3·00	
	1	Hg_I	3·22	
	1	Hg_{II}	2·95	
	2	Mn	2·92	
	2	Mn	3·02	
Hg_{II}	4	Hg_I	2·95 Å	2·95 Å
	2	Hg_{II}	3·00	
	4	Mn	2·92	

* See Fig. 2.

6. Discussion of the structure

(i) *General features*

The very short *c* repeat distance could account for both the uncommon fibrous habit and the ease of cleavage. The formation of manganese chains parallel to the *c*-axis is also interesting; the short separation distances (3·00 Å) might be expected to give rise to magnetic interactions between nearest neighbours. The magnetic behaviour of the compound is unusual (De Wet, 1955); although the interactions are not fully understood yet, they may well provide the key to the architecture of the structure (De Wet, 1960).

The packing arrangement of the mercury atoms leads to large voids in the structure. Those situated, for example, at the positions $(0, 0, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, producing channels along the 4-fold axes, could accommodate spheres with diameter 0·732 times the mercury diameter (compare, e.g., with the voids in the close-packed structures). The overall packing density in Mn_2Hg_5 is, however, still high, the structure containing about 36% voids as compared to 26% in the close-packed structures.

The striking similarity between this structure and that of a co-ordination complex, $Pd(NH_3)_4Cl_2.H_2O$ (Dickinson, 1934), is an occurrence apparently without parallel among the metallic structures [Fig. 1(*a*), (*b*)]. The structures also differ in important respects: the set of special positions occupied by the palladium atoms are left as vacancies in the Mn_2Hg_5 structure (the voids referred to above). Furthermore, the atomic layers in the complex (at $z=0$) are, due to the size of the chloride ions, not in contact.

(ii) *Co-ordination geometry*

The essential features of the Mn_2Hg_5 structure, as well as its relationship to other alloy structures, may be more readily appreciated if it is analyzed along the lines developed by Frank & Kasper (1958, 1959). By dissecting the complex alloy structures into simpler geometrical forms, such as the 'major skeleton', 'primary' and 'secondary' layers, they have demonstrated in an elegant fashion how these structures arise from space-filling arrangements of co-ordination polyhedra. Although the structures treated by them are all characterized by a high density of tetrahedral sites, resulting in co-ordination polyhedra with triangular faces—features which do not obtain in the Mn_2Hg_5 structure—the application of certain of their concepts to this structure is nevertheless illuminating.

Consider, first of all, the co-ordination around the manganese atoms (Fig. 2). It is 12-fold, a common number for metals, but unlike the co-ordination types hitherto observed, namely, the cuboctahedron of the close-packed structures and the icosahedron of the transition metal alloys. The co-ordination polyhedron is a pentagonal prism-bipyramid, in which the manganese atoms occupy the apices of the bipyramid, and mercury atoms the remaining apices. Since the Mn–Hg

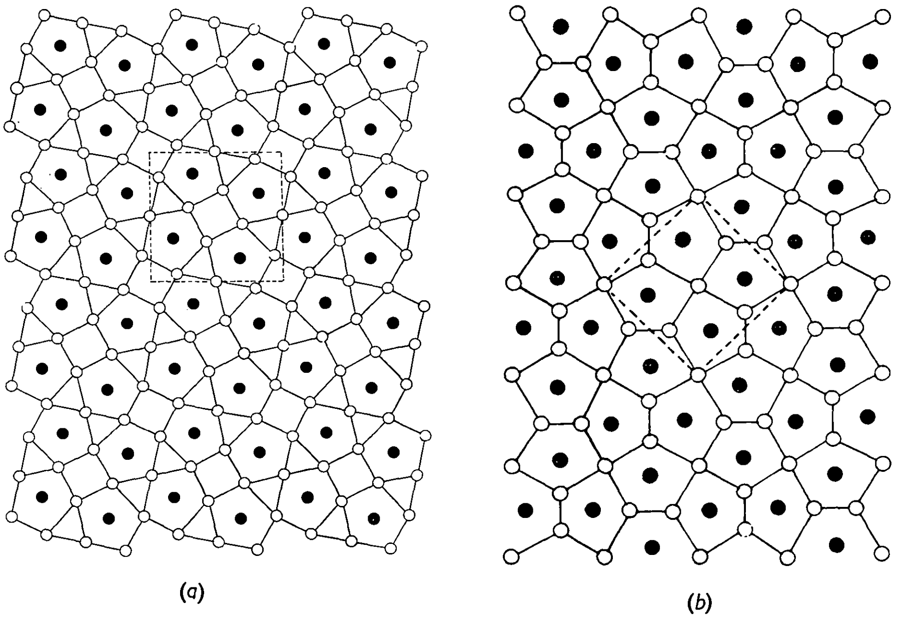

Fig. 3. Two tetragonal structures in which the tessellations of the primary layers (open circles) result from the packing of pentagons. The secondary layers, at $z = \frac{1}{2}$, form a $3^2.4.3.4$ net. (*a*) The structure of Mn_2Hg_5, in which the primary layer consists of pentagons sharing corners. (*b*) The structure of Si_2U_3, in which the primary layer consists of pentagons sharing sides.

bond lengths are all equal to within 10% (Table 4), this polyhedron may be related to the icosahedron in a simple way: twinning through 180°, along a plane situated half-way between the two coplanar groups of 5 atoms, transforms one polyhedron into the other. The manganese co-ordination may therefore be represented by a *twinned icosahedron.*

It is evident that the structure may also be dissected into primary and secondary layers. The primary layer, regarded as a tessellation of pentagons, squares and triangles, is shown in Fig. 3(*a*); the secondary layer of manganese atoms forms a simple $3^2.4.3.4$ tessellation.* The primary layer is, at first sight, complex, as it involves three types of polygon and two types of vertex, 5.3.5.4 and 5.3.5.3. Closer examination reveals that the net simply consists of pentagons packed in such a way that each shares its corners with neighbouring pentagons, without sharing sides.

The Mn_2Hg_5 structure may therefore be visualized as an arrangement of twinned icosahedra, stacked edge-to-edge in the second closest type of planar packing ($3^2.4.3.4$) and interpenetrating in the *c*-direction. The question arose whether this was the closest possible packing arrangement of such icosahedra; in other words, whether a more closely packed tessellation of pentagons, with their centres in $3^2.4.3.4$ array, exists. Such a tessellation could, indeed, be constructed [Fig. 3(*b*), open circles]; here each pentagon shares all its sides with five equidistant neighbours, and corners with two further ones. The composition of an alloy consisting of *B* atoms in this array, interleaved with layers of *A* atoms in $3^2.4.3.4$ array, would be A_2B_3. This *B*-tessellation is, however, only possible if the pentagons have a specific shape, namely, with four equal sides and one with length 0·7 times that of the other, and with three angles of 120° and two of 90°. The inequality in bond lengths gives rise to unfavourable packing for spheres of equal size, and this may be why the composition Mn_2Hg_3 is not preferred. It is interesting to note that a structure with this atomic arrangement, but with a different allocation of sites, exists, namely that of Si_2U_3 (Zachariasen, 1949) and the isostructural Al_2Th_3 (Braun & Van Vucht, 1955). The packing problem in the primary layers is overcome by the equal distribution of both types of atom over the primary layer sites [open circles, Fig. 3(*b*)], while the remaining actinide atoms occupy the secondary layer sites [black dots, Fig. 3(*b*)]. In Si_2U_3, for example, the Si atoms occupy the terminal sites of the short bonds in the primary layer, forming Si_2 islands, while the U atoms occupy the remaining sites in the two layers. The most significant fact, however, is that the actinide atoms in the secondary layers possess the same, if somewhat distorted, co-ordination symmetry as that of manganese in Mn_2Hg_5. It is peculiar that these two structure types are apparently the only alloy structures known to crystallize in the space group *P*4/*mbm* (cf. Pearson, 1958).

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* It is remarkable how frequently secondary layers assume the $3^2.4.3.4$ tessellation (cf. Frank & Kasper, 1959).

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Die Verfeinerung der Kristallstruktur von Kröhnkit, $Na_2Cu(SO_4)_2 . 2H_2O$

VON B. RAMA RAO*

Mineralogisch-Kristallographisches Institut der Universität Göttingen, Lotzestr. 16–18, *Deutschland*

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The crystal structure of kroehnkite has been refined by Fourier- and difference-syntheses. Cu shows a (4 + 2) octahedral coordination, with two oxygen atoms and two H_2O groups forming a square planar coordination. The interatomic distances between Cu and its neighbours in the coordination polyhedron are: $Cu–H_2O = 1·95$ Å (2 ×); $Cu–O_{III} = 1·99$ Å (2 ×) and $Cu–O_{II} = 2·41$ Å (2 ×). The S–O and O–O distances in the sulphate tetrahedron are of the usual order of magnitude. Sodium has sevenfold coordination. From a consideration of the interatomic distances and angles it is concluded that there may exist hydrogen bonds between the H_2O groups and the sulphate tetrahedra. The final R values obtained are: $R_{[001]} = 0·07_6$ and $R_{[100]} = 0·09_5$; if the unobserved reflexions are included the following R values are obtained: $R'_{[001]} = 0·08_1$ and $R'_{[100]} = 0·10_0$.

Einleitung

Die Kristallstruktur von Kröhnkit wurde von Dahlman (1952) und Leone & Sgarlata (1954) bestimmt. Beide Strukturen sind prinzipiell gleich, aber die Parameter und die strukturellen Einzelheiten sind erheblich verschieden. Zum Vergleich zeigt Tabelle 1 die Parameter, die Dahlman und Leone & Sgarlata erhielten. Im Rahmen einer systematischen Untersuchung von Kristallstrukturen blauer Cu^{2+}-Verbindungen im hiesigen Institut (vgl. Mazzi, 1955; Gattow, 1958; Gattow & Zemann, 1958; Bachmann & Zemann, 1960) ist nun die Kristallstruktur des Kröhnkits verfeinert worden, um die Parameter genauer zu bestimmen und die strukturellen Einzelheiten zu prüfen.

Kröhnkit, $Na_2Cu(SO_4)_2 . 2H_2O$ kristallisiert monoklin prismatisch in der Raumgruppe $P2_1/c(C_{2h}^5)$ mit zwei Formeleinheiten in der Elementarzelle. Die Gitterkonstanten der früheren Arbeiten sind:

	Dahlman	Leone & Sgarlata	Palache (1939) (morphologisch)
a_0	5,78 Å	5,78 Å	
b_0	12,58 Å	12,62 Å	
c_0	5,48 Å	5,46 Å	
β	108° 30′	106° 40′	108° 30′
$a_0:b_0:c_0$	0,4594 : 1 : 0,4356	0,4580 : 1 : 0,4326	0,4586 : 1 : 0,4357
Dichte	2,95 g.cm.$^{-3}$ (berechnet)	2,89 g.cm.$^{-3}$ (berechnet)	$2,90 \pm 0,02$ g.cm.$^{-3}$ (gemessen)

Gitterkonstanten und Raumgruppe

Äquimolekulare Mengen von $CuSO_4 . 5H_2O$ und Na_2SO_4 wurden in möglichst wenig destilliertem Wasser gelöst; die Lösung wurde schwach erwärmt und dann bei 40 °C. eingeengt (Dana, 1951). Nach 24 Stunden schieden sich gut ausgebildete kleine Kristalle von Kröhnkit aus.

Äquator-Weissenberg-Aufnahmen um [001] und [100] mit Cu $K\alpha$-Strahlung wurden aufgenommen und die Gitterkonstanten aus den äusseren Reflexen bestimmt. Der Winkel β wurde einer Precession-Aufnahme um [010] mit Mo $K\alpha$-Strahlung ($\mu = 30°$) entnommen. Die Gitterkonstanten sind:

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* Jetzige Adresse: Regional Research Laboratory, Hyderabad 9, India.