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THE STRUCTURE OF $BaCl_2, 2H_2O$

BY

AKSEL TOVBORG JENSEN

KØBENHAVN
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INTRODUCTION

The structural differences between $CuCl_2, 2\,H_2O$[1] and $SrCl_2, 2\,H_2O$[2] are readily explained by the fact that the bonds of the Cupric ion are directional while the bonds of the Strontium ion are not. The reason why there exist a considerable number of different structures of compounds $AX_2, 2\,H_2O$ (A being an alkaline earth metal, X a halogen) is less obvious. Usually a compound type with only one "variable", the radius ratio $\frac{R_{cation}}{R_{anion}}$, is not expected to exhibit such a variety of different crystal structures. However, it must be borne in mind that R_{H_2O} is probably constant, so that we have two variables, $\frac{R_{cation}}{R_{anion}}$ and $\frac{R_{anion}}{R_{H_2O}}$, each of which on alteration tend to alter the structure. In other words, we have a definition interval which is a rectangle and not a straight line. The only way to an understanding of the dynamics of a group of compounds is through a detailed knowledge of their geometry. The present paper and the preceding one[2] provide this knowledge for two points of the definition interval, but investigations of several other points would be desirable.

X-ray investigations on $BaCl_2, 2\,H_2O$ were commenced by Náray-Szabó and Sasvári,[3] who abandoned it. After a considerable amount of labour the present author also had to leave the problem unsolved. The complete structure of $SrCl_2, 2\,H_2O$[2], however, shed some fresh light on it, and by utilizing all the scattered data and some new ones it proved possible to determine the complete structure of $BaCl_2, 2\,H_2O$.

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[1] D. Harker, Z. Krist. **93** (1936) 136.

[2] A. Tovborg Jensen. D. Kgl. Danske Vidensk. Selskab, Mat.-fys. Medd. XX (1942) Nr. 5.

[3] St. v. Náray-Szabó and K. Sasvári, Z. Krist. **97** (1937) 235.

Crystallography of $BaCl_2, 2H_2O$.

The crystal class of $BaCl_2, 2H_2O$ was shown by Wyrouboff and Groth[1] to be 2/m (C_{2h}), the monoclinic holohedral class. The space group was found by Náray-Szabó and Sasvári to be $P2_1/n\,(C_{2h}^5)$. The systematic absences in diagrams indexed by the author are in agreement with $P2_1/n$, and the structure finally arrived at proves the assignment of $BaCl_2, 2H_2O$ to the holohedral class to be correct.

The space group C_{2h}^5 in the orientation $P2_1/n$ has the following special points:

$$2\colon\ (a)\ 000;\ \frac{1}{2}\frac{1}{2}\frac{1}{2}$$

$$(b)\ \frac{1}{2}00;\ 0\frac{1}{2}\frac{1}{2}$$

$$(c)\ \frac{1}{2}\frac{1}{2}0;\ 00\frac{1}{2}$$

$$(d)\ \frac{1}{2}0\frac{1}{2};\ 0\frac{1}{2}0$$

and the general point

$$4\colon\ (e)\ xyz;\ \bar{x}\bar{y}\bar{z};\ \frac{1}{2}+x,\ \frac{1}{2}-y,\ \frac{1}{2}+z;\ \frac{1}{2}-x,\ \frac{1}{2}+y,\ \frac{1}{2}-z.$$

The structure factor is

$$A = 4\cos 2\pi\left(hx + lz + \frac{h+k+l}{4}\right)\cos 2\pi\left(ky - \frac{h+k+l}{4}\right)$$

$$B = 0$$

separated

$$\begin{array}{r|l} h+k+l = 2n & A = -4\cos 2\pi(hx+lz)\cos 2\pi ky \\ & B = 0 \\ h+k+l = 2n+1 & A = -4\sin 2\pi(hx+lz)\sin 2\pi ky \\ & B = 0. \end{array}$$

The lattice constants given in[2] and a set of accurate values obtained by the author are given in Table 1. The agreement is

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[1] Gmelins Handbuch d. anorg. Ch. System Nr. 30. Ba.

[2] St. v. Náray-Szabó and K. Sasvári. Z. Krist. 97 (1937) 235.

good. The second set is considered the more accurate, since they are determined from powder photographs (Phragmén focussing camera and circular Bradley camera, 191 mm. diameter), while the first set are from oscillation photographs.

$BaCl_2, 2H_2O$ is the well known hydrate of $BaCl_2$. $BaCl_2, H_2O$ has never been obtained from an aqueous solution. KIRSCHNER ([1] p. 180) prepared $BaCl_2, H_2O$ by treating solid $BaCl_2, 2H_2O$ with methyl alcohol. The solubility curve of $BaCl_2, 2H_2O$ is known from the cryohydratic point $-7.8°$ and upwards. The temperature at which this curve and the solubility curve of the lower hydrate (monohydrate) intersect is not known, but is has been stated to be above 60° C. *Vide*[1] p. 180. Incidentally this temperature has been found to lie between 108° and 110° C., in the course of experiments to prepare mixed crystals of $BaCl_2, 2H_2O$ and $BaBr_2, 2H_2O$ with a maximum of $BaBr_2, 2H_2O$. Below 108° C. crystals of $BaCl_2, 2H_2O$ under mother liquor will keep indefinitely; above 110° C., they deteriorate rapidly.

Catalogues of Reflections.

The following lists of reflections were applied in deducing the structure.

(1) Complete set of 30° oscillation diagrams of [001] zone, camera diameter 100 mm, CuK_α radiation.

(2) Complete series of 30° oscillation diagrams of [100] zone, FeK_α radiation.

(3) hk0, hk1, h0l, h1l, h2l, h3l Weissenberg diagrams, Buerger goniometer, CrK_α radiation.

(4) Full rotation photograph of a cylindrical crystal, [001] axis.

(5) Powder photographs, Phragmén focussing camera, CrK_α and K_β radiation. Powder photograph, CoK_α radiation, circular camera 191 mm. diameter.

(1) and (2) were indexed by Bernal's method.

The equatorial intensities of (1), (2), and (4) were used for Fourier syntheses. (3) afforded an easy check on the space group, (5) were used for lattice constant determination, and the intensities applied to check the complete structure.

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[1] GMELINS Handbuch d. anorg. Ch. System Nr. 30. Ba.

Fourier syntheses.

The difficulties in determining the complete structure of $BaCl_2, 2\,H_2O$ already realized by Náray-Szabó and Sasvári[1] are easily seen. The Ba atom contains so many electrons that it obscures the Cl and O atoms. The number of electrons in Ba^{++}, Cl^{-} and O are 54, 18, and 8, or as 100: 32 : 15. At high reflection angles the effective numbers of electrons in Cl^{-} and O are even smaller fractions of the number for Ba^{++}. At $\sin\theta/\lambda = 0.5$ the figures are 100 : 25 : 8. These figures pertain to atoms at rest. At room temperature the figures are still more unfavourable since thermal movements tend to decrease the effective number of electrons in lighter atoms more strongly than in heavy ones.

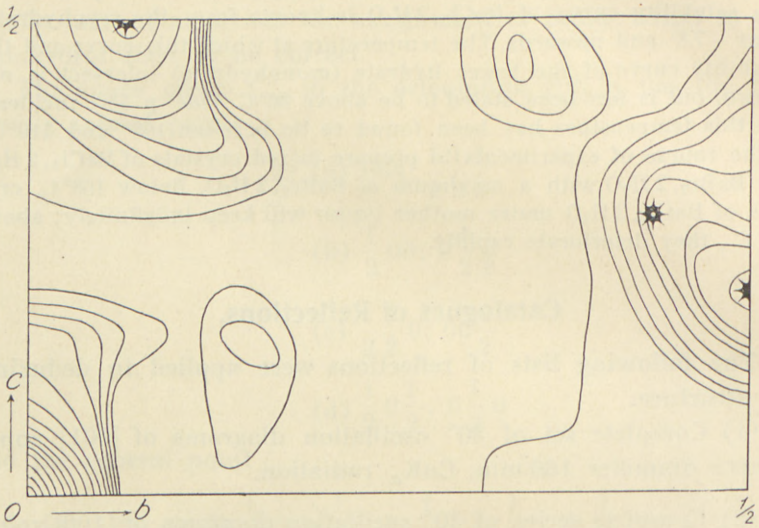

Fig. 1. Patterson-Fourier projection on 100 in $BaCl_2$, $2\,H_2O$. Visually estimated intensities. Ba-Ba peaks shown as stars.

The observed spot intensities hk0 and 0hk were converted into series of approximate F's by the aid of appropriate charts. Such charts are described in.[2]

Patterson-Fourier projections on 100 and 001 were computed and drawn (Fig. 1 and Fig 3). Fig. 2 shows the projection unit, its symmetry elements and the calculation area in the two strictly analogous cases. The space group $P\,2_1/n\,(C_{2h}^5)$ projects

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[1] St. v. Náray-Szabó and K. Sasvári, Z. Krist. 97 (1937) 235.

[2] A. Tovborg Jensen, D. Kgl. Danske Vidensk. Selskab, Mat.-fys. Medd. XX (1942) Nr. 5.

on to 100 as well as on 001 in the plane group Pba, *vide*[1] and [2]. An atomic arrangement of Pba symmetry gives a Patterson vector map of Pmm symmetry.

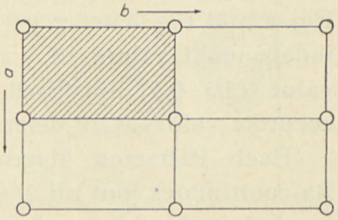

Fig. 2. Unit of projection and symmetry elements in 100 and 001 Patterson-Fourier projections in $BaCl_2, 2\,H_2O$. Shaded: area of calculation.

The Ba-Ba peaks on Fig. 1 and Fig. 3 are very conspicuous and easily found. It is seen at once from the figures that the Ba atom is in general position. The special two-fold positions 00, $\frac{1}{2}\frac{1}{2}$ and $\frac{1}{2}0$, $0\frac{1}{2}$ are ruled out. Atoms at these special positions should give rise to peaks in the vector map at 00 and $\frac{1}{2}\frac{1}{2}$, and the vector maps contain no outstanding peak at $\frac{1}{2}\frac{1}{2}$.

One atom in general position xy; $\frac{1}{2}-x$, $\frac{1}{2}+y$; $\bar{x}\bar{y}$; $\frac{1}{2}+x$, $\frac{1}{2}-y$ produces a set of peaks situated as shown in Fig. 4.

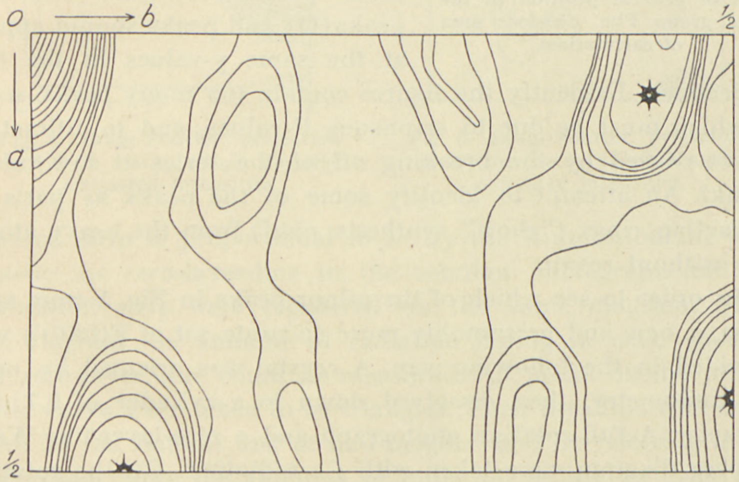

Fig. 3. Patterson-Fourier projection on 001 in $BaCl_2$, $2\,H_2O$. Visually estimated intensities. Ba-Ba peaks shown as stars.

Fig. 1 and Fig. 3 correspond exactly to Fig. 4, and finally prove the Ba atom to be in general position. Ba-coordinates found from

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[1] A. L. Patterson, Z. Krist. **90** (1935) 543

[2] W. L. Bragg and H. Lipson, Z. Krist. **95** (1936) 323.

Fig. 1 and Fig. 3 are x, y = 0.04, 0.22; y, z = 0.22, 0.15. The two independent values of y agree, but are rather different from the value 0.16—0.17 surmised by Náray-Szabó and Sasvári.[1] More accurate values were determined later.

Each Patterson diagram yields 4 different sets of the two Ba-coordinates, but all 4 sets are really identical, differing only in choice of origin and axis orientation.

The Ba-coordinates obtained suffice to fix the signs of all reflections. With the F values already employed and the signs now obtained the corresponding Bragg-Fourier projections were computed. They are shown in Fig. 5 and Fig. 6. Heavy Ba atoms appear where they were expected, but the remaining peaks are not capable of immediate interpretation. The projection area, one quarter of the unit cell, should contain two medium peaks (Cl), and two low peaks (O), and peaks should appear at the same y-values in the two projections. Evidently the figures contain too many peaks, some of which must be due to erroneous F-values, and to diffraction effects caused by the breaking off of the series at low values of hkl. An attempt to identify some of the peaks as parts of diffraction rings ("ghost"-synthesis, *vide*[2]) from the heavy atoms was without result.

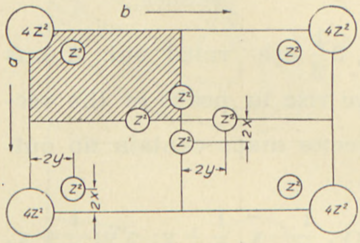

Fig. 4. Interatomic vectors (Patterson peaks) corresponding to one atom in general position in the plane group Pba. Shaded: area of calculation.

In order to see which of the minor peaks in Fig. 5 were spurious, a new and presumably more accurate set of F(hk0)'s was provided in the following way. A crystal was oriented by optical goniometry, then dissolved down to a cylinder of 0.7 mm. diameter. A full rotation photograph and a zero-layer-line Weissenberg diagram were taken with Cu-radiation. On the rotation photograph a calibration strip was printed by exposing the film to the direct beam through a rotating desk in which is cut a sector limited by a radius and a logarithmic spiral curve. The amount of radiation falling at a distance X from the end of the

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[1] St. v. Náray-Szabó and K. Sasvári, Z. Krist. 97 (1937) 235.

[2] A. Tovborg Jensen, D. Kgl. Danske Vidensk. Selskab, Mat.-fys. Medd. XX (1942) Nr. 5.

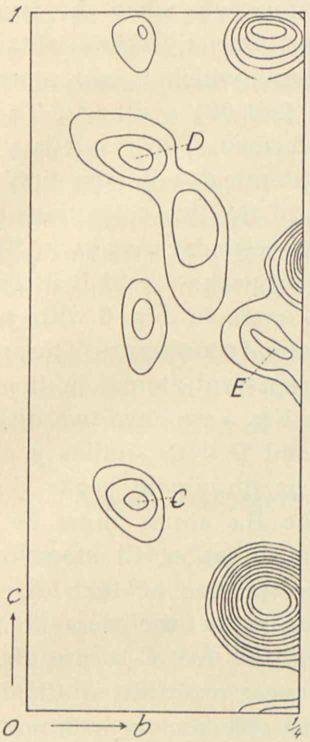

Fig. 5. Bragg-Fourier projection on 100 in $BaCl_2$, 2 H_2O. Visually estimated intensities.

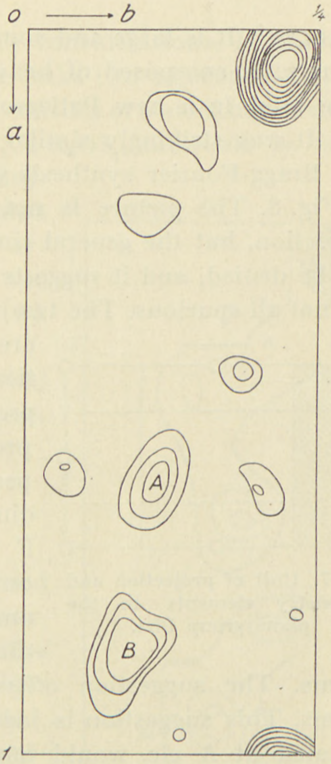

Fig. 6. Bragg-Fourier projection on 001 in $BaCl_2$, 2 H_2O. Visually estimated intensities.

exposed strip is proportional to X. By the Kipp automatic photometer the zero-layer-line in the rotation photograph and the calibration strip were registered on the same diagram. From this diagram the amount of radiation falling in each spot on the zero-layer line could be measured. All peaks on the photometer curve were taken to be triangles. Their breadths were measured at the bottom and at half heights, and by referring to the calibration curve the amounts of radiation falling on each spot were calculated in arbitrary units. The amounts of radiation were divided by the polarisation and Lorentz factors and the absorption factor. The quotient gives $F^2(hk0)$ in arbitrary units. The polarization and Lorentz factors were taken from *Internationale Tabellen zur Bestimmung von Kristallstrukturen* p. 567. The absorption factor was calculated according to

Bradley[1]. It is large and somewhat uncertain when the crystal, as here, is composed of heavy atoms. The $F^2(hk0)$'s obtained were used in a new Patterson synthesis which is not reproduced. It was strikingly similar to the first 001 synthesis. Then a 001 Bragg-Fourier synthesis was performed. The result is given in Fig. 8. The picture is not quite identical with the first 001 projection, but the general similarity of the two projections cannot be denied, and it suggests that the secondary peaks in Fig. 6 are not all spurious. The two prominent peaks A and B in Fig. 6 are found again in Fig. 8 with practically identical coordinates. They most probably represent atoms. In the 100 projection Fig. 5 we have two distinct peaks C and D with similar y coordinates. The prominent peaks E and F near the Ba atoms must be left out of consideration. Cl atoms at E and F irrespective of their X-coordinates would be too near the Ba atoms. The suggestion offers itself, that A-B-C-D are the Cl atoms. This suggestion is made the more probable as Cl atoms situated at A etc. would have reasonable distances from two adjacent Ba atoms (whose coordinates we know accurately). The proposed Cl atoms would link the Ba atoms in sheets parallel with the developed face of our crystal. A similar arrangement has previously been found in $SrCl_2, 2\,H_2O$.

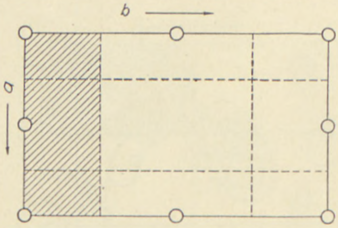

Fig. 7. Unit of projection and symmetry elements in the plane group Pba.

A calculation showed that this arrangement of Cl atoms would also explain quite nicely all secondary peaks in the 001 Patterson projection as due to interaction between Ba and Cl.

The projections discussed give few or no indications of the O-coordinates. The projection Fig. 8, which must be considered more accurate than Fig. 5 and Fig. 6, however, seems to indicate that O atoms must be somewhere on the "high ground" in the upper half of the picture.

A model to scale of the proposed structure was built of plasticine and glass rods. Combination of the two projections to a structure in space involves no difficulties. The model suggested one and only one position for each of the water molecules rea-

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[1] A. J. Bradley, Proc. Phys. Soc. **47** (1935) 879.

sonably to be expected from space considerations. In the positions suggested each water molecule links two adjacent Ba atoms.

The entire atomic arrangement consists of a stacking of sheets. Each sheet is a complete $(BaCl_2, 2\,H_2O)_{n^2}$ molecule as far as geometrical aspects are concerned. $SrCl_2, 2\,H_2O$ previously investigated contains similar sheets, but the arrangement of H_2O and Cl around the metal atoms is different in the two cases.

A preliminary calculation of 0kl intensities showed satisfactory agreement with the observed values.

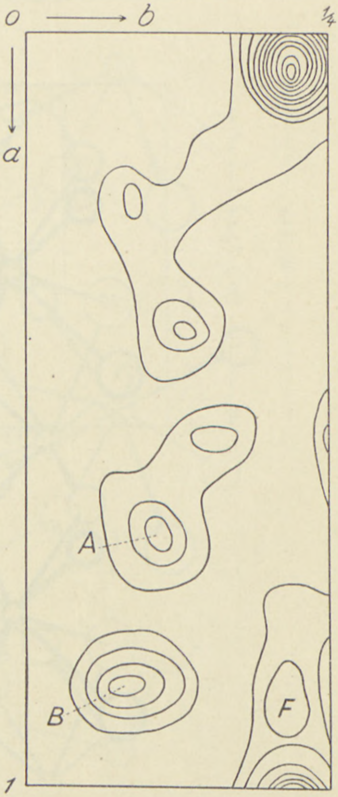

Fig. 8. Bragg-Fourier projection on 001 in $BaCl_2, 2\,H_2O$. Photometric intensities.

Atomic Parameters.

Before subjecting the proposed structure to the final test of comparing calculated and observed intensities of the general type hkl, the best values of atomic parameters were selected. Parameter values from different projections are undoubtedly of varying accuracy. All intensities employed are not equally accurate, thus data with Cu radiation are to be preferred to Fe radiation data. Photometric estimation is considered better than visual estimation. But it is not easy to see which of the two independent sets of values obtained from each Patterson diagram is the better, nor to estimate whether figures obtained by Patterson synthesis are more accurate than the slightly different values obtained from subsequent Bragg synthesis on the same data. Hence it was decided to take for final values the averages from all projections. The figures and averages are given in Table 2. Table 2 gives some idea of the accuracy which may be attached to the averages. Each set of parameter values has been obtained from a carefully drawn detail map of the peak in question. These maps, 15 in all, are not reproduced.

The final water parameters were chosen in the following way. It was assumed that the water molecules link two Ba atoms at distances of about 2.85 Å, and that all distances from other neighbouring atoms are not much below the sums of corresponding radii. A few trials gave parameters involving reasonable distances from all neighbouring atoms and causing the water molecule to make two distinct contacts with Cl atoms apart from the two contacts with Ba atoms originally assumed. Four such contacts, two negative and two positive, show that the water molecule is of Bernal's "tetrahedral" type.[1]

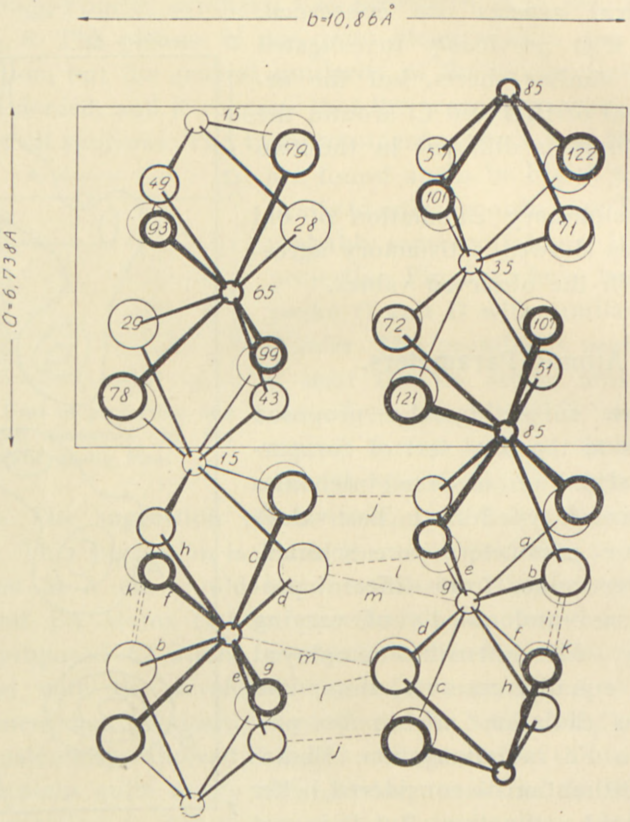

Fig. 9. $BaCl_2, 2H_2O$ projected on 001. ○ Ba, ◯ H_2O, ◯ Cl.

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[1] J. D. Bernal and R. H. Fowler. J. chem. Phys. 1 (1933) 515.

The atomic parameters are tabulated in Table 3. Interatomic distances are given in Table 4. The distances in the last column of Table 4 are the corresponding radius sums.

The letters in the first column of Table 4 refer to Fig. 9 and

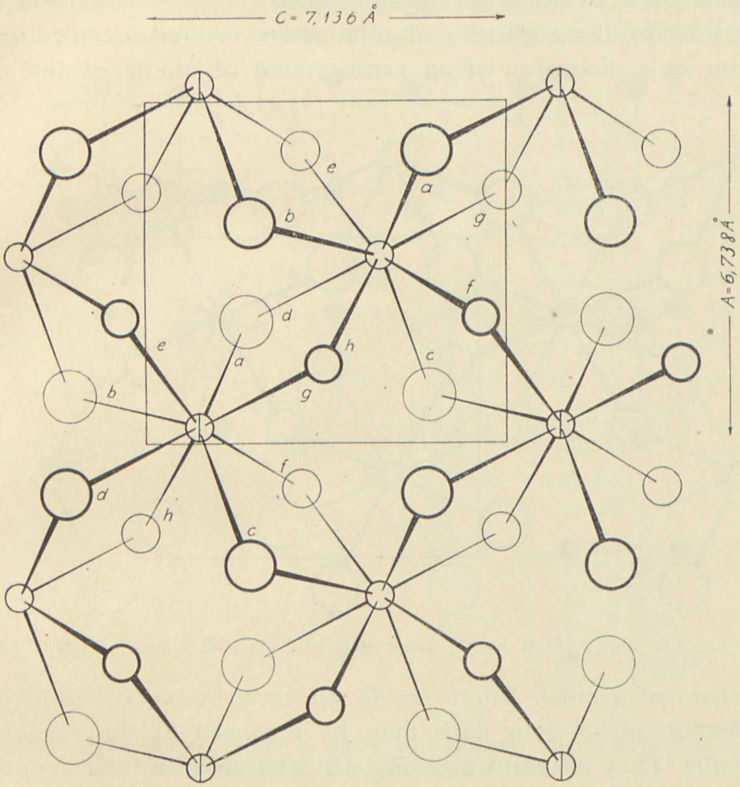

Fig. 10. $BaCl_2, 2\,H_2O$. Single layer projected on 010.
⦶ Ba above plane of drawing. ○ Ba below plane of drawing. ○ H_2O. ◯ Cl.

Fig. 10, which depict the structure. It is scarcely possible to denote all the distances in a complicated structure like the one in hand, in such a way that their position in space can be visualized without the aid of a diagram or a model.

Description of the Structure.

The structure consists of identical $(BaCl_2, 2\,H_2O)_{n^2}$ layers of which one is shown in Fig. 10. The layer is projected on

010. The figure should be compared with Fig. 11, the corresponding picture of a $(SrCl_2,\ 2\,H_2O)_{n2}$ layer which is taken from the preceding paper.[1] The two layers are similar in so far as a metal atom in each is surrounded by 4 Cl and 4 H_2O. The chief difference between a Ba layer and a Sr layer is best seen by considering these clusters of eight atoms around a central metal atom as a distortion of an arrangement of atoms at the eight corners of a cube. There are in all seven ways in which two different sets of four balls may be arranged at the corners of a cube. They are shown in Fig. 12 denoted with their symmetry symbols in the Hermann-Mauguin shorthand.

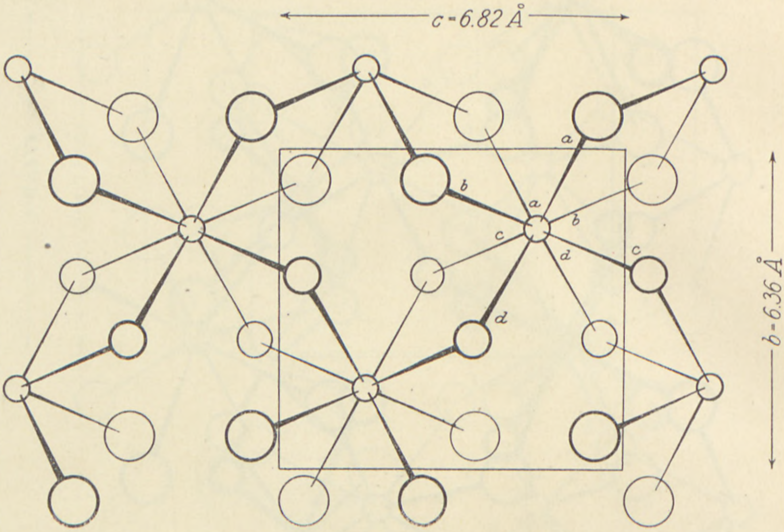

Fig. 11. $SrCl_2,\ 2\,H_2O$. Single layer projected on 100. ○ Sr, ○ H_2O, ○ Cl.

The $SrCl_2,\ 2\,H_2O$ layer is built by distortion and linking of 4mm units, while $BaCl_2,\ 2\,H_2O$ is derived from mmm units. Possibly several others of these arrangements may be found in other crystals of AX_2Y_2 compounds built of neutral layers, or even in crystals containing electrically charged layers of this formula.

Another noteworthy difference between the two kinds of layer is that while in $SrCl_2,\ 2\,H_2O$ the Sr atoms of one layer all lie in a plane, in $BaCl_2,\ 2\,H_2O$ they form a puckered layer. This puckering causes each Ba atom to be rather close to one Cl

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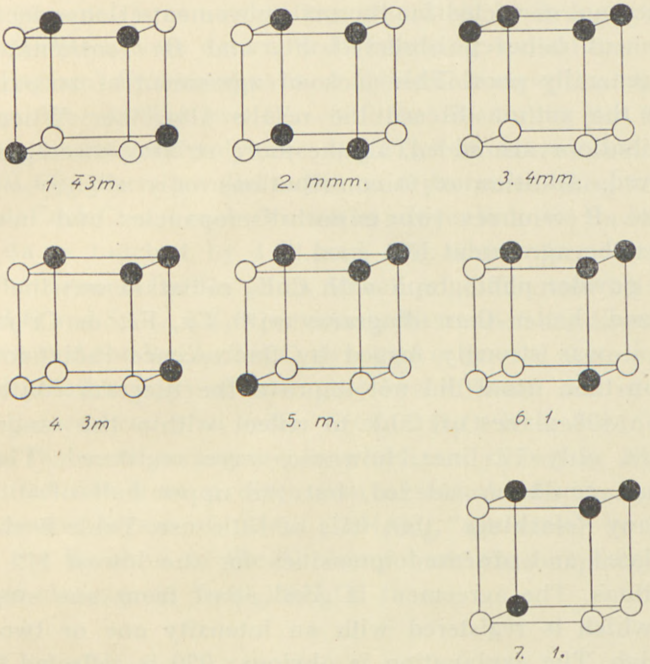
[1] A. Tovborg Jensen, D. Kgl. Dansk Vidensk. Selskab, Mat.-fys Medd. XX (1942) Nr. 5.

atom in the adjacent layer. The corresponding line is called m in Fig. 9. The distance is 3.38 Å as compared with 3.20 for a contact. A similar feature is not present in $SrCl_2$, 2 H_2O, where Sr atoms on all sides are completely screened by adjacent Cl and H_2O.

The distances between atoms in adjacent layers in $SrCl_2$, 2 H_2O were all well above the corresponding radius sums. In $BaCl_2$, 2 H_2O several distances between Cl atoms and H_2O molecules in different layers are equal to the corresponding radius sum. Hence the electrostatic attraction between adjacent layers is probably considerable. This attraction seems to be the reason why $BaCl_2$, 2 H_2O although a layer lattice, does not easily cleave parallelly to the layers.



1. $\bar{4}3m$.
2. mmm.
3. 4mm.
4. 3m
5. m.
6. 1.
7. 1.

Fig. 12. The seven different ways in which two different sets of four balls may be arranged at the corners of a cube.

Comparison between Calculated and Observed Intensities.

Table 5 gives a comparison between observed and calculated values of F(hk0). The observed F's are the set photometrically registered. They are given in the arbitrary units in which they were obtained. The calculated values employ the final set of parameters as given in Table 2. The f curves applied were James's and Brindley's. The agreement is considered satisfactory. Observed F's at high glancing angles are much lower than the calculated values in accordance with the fact that the calculated F's are not corrected for thermal movement (Debye factor). The agreement between observed F's and *Ba contributions alone* was generally poor. This lack of agreement at an early stage made the author discard the results altogether. When the Cl contributions are added, all the more striking discrepancies are removed. Addition of O contributions only slightly alters the picture. It removes two minor discrepancies and in no case makes the agreement less good.

A powder photograph with CoK_α radiation was the best one obtained, better than diagrams with Cu, Fe, or Cr radiation. Still, it was strongly fogged by fluorescence radiation. Lower tension than usual did not improve the diagram. With Co radiation 408 planes are able to reflect within the range of the camera, only 77 lines, however, were registered. The entire diagram could be indexed, but the upper half of it contains so many "clashings" that it is of little use. Table 6 shows the calculated and observed intensities for the lowest 112 possible reflections. The agreement is good apart from one single line, 020, which is registered with an intensity one or two classes too high. The explanation is obvious: 020 is reflected from the only face developed on small flaky crystals and hence apt to give too strong reflections because of preferential orientation in the powder specimen. The $BaCl_2, 2\,H_2O$ powder had been precipitated from a strong aqueous solution by alcohol. No attempt was made to remove the effect by grinding the powder. Moderate grinding of soft hydrate crystals spoils the quality of their powder-diagram. As previously noted for the hk0 intensities, it was seen that the Ba contribution alone is quite insufficient to account for the observed intensities. The Ba and Cl contributions suffice, and the O contributions make but little difference.

Summary.

The complete structure of $BaCl_2, 2\,H_2O$, which is determined by 15 independent parameters, has been worked out by an extensive use of Patterson- and Bragg-Fourier-synthesis on visually and photometrically estimated intensities. Ba parameters were determined very accurately by Patterson and Bragg synthesis, Cl parameters somewhat less accurately by Bragg synthesis. O parameters were determined (following indications on a Fourier diagram) by consideration of plausible coordination and space requirement. The two O's could be fitted into the $BaCl_2$ framework in one and only one way. The structure consists of $(BaCl_2, 2\,H_2O)_{n^2}$ layers parallel to the most prominent face, 010, of the crystal. Each Cl and each O atom in a layer link two Ba atoms, so each Ba is touched by 4 Cl and 4 O, which form a compact cluster around the Ba atom. Structural differences between $BaCl_2, 2\,H_2O$ and $SrCl_2, 2\,H_2O$ previously determined are discussed. It is shown that the $BaCl_2, 2\,H_2O$ structure is derived from one of the seven possible ways of arranging two different sets of four balls at the corners of a cube. $SrCl_2, 2\,H_2O$ is derived from another of the seven arrangements, which are shown in Fig. 12 It is pointed out from a discussion of atomic distances that the consecutive layers of $(MeCl_2, 2\,H_2O)_{n^2}$ are closer to each other in the Ba than in the Sr compound. This explains the absence of cleavage in $BaCl_2, 2\,H_2O$.

Acknowledgements.

I am highly indebted to Professor Niels Bjerrum for his unfailing interest in these studies and for the excellent working conditions in the laboratory; to Professor Gunnar Hägg of Uppsala, in whose laboratory part of the work was done in the spring of 1940, for his constant aid and encouragement, and to the Carlsberg Foundation and K. A. Larssens Legat for grants.

Copenhagen.
Royal Veterinary and Agricultural College.
Chemical Laboratory.

Table 1.

Lattice constants of $BaCl_2$, 2 H_2O.

a	b	c	β	
6.69 Å	10.86 Å	7.15 Å	91°.05	(Náray-Szabó and Sasvári)
6.738 Å	10.86 Å	7.136 Å	90°.57	(Author)

Table 2.

All parameter values obtained and their averages.

	Fig. 1 a	Fig. 3 a	Fig. 3 b	X a	X b	Fig. 5	Fig. 6	Fig. 8	Average
Ba x . . .	. .	0.050	0.037	0.050	0.042	. .	0.047	0.043	0.045
y . . .	0.216	0.217	0.219	0.216	0.215	0.217	0.218	0.218	0.217
z . . .	0.145	. .	. .	. .	. .	0.150	. .	. .	0.147
Cl_I x . . .	. .	. .	. .	. .	. .	. .	0.838	0.864	0.851
y . . .	. .	. .	. .	. .	. .	0.087	0.088	0.077	0.084
z . . .	. .	. .	. .	. .	. .	0.781	. .	. .	0.781
Cl_{II} x . . .	. .	. .	. .	. .	. .	. .	0.622	0.660	0.641
y . . .	. .	. .	. .	. .	. .	0.094	0.113	0.107	0.105
z . . .	. .	. .	. .	. .	. .	0.289	. .	. .	0.289

The columns marked a contain values read off from special point peaks in the Patterson diagrams. Values in columns marked b are read off from general point peaks. There are no Fig. 1 b data, because the general point peak in Fig. 1 is too near a special point peak and too blurred to be of any use. X a and X b are from a Patterson x-y diagram based on photometric data, which is not reproduced.

Table 3.

Atomic parameters in $BaCl_2$, 2 H_2O.

	x	y	z
Ba	0.045	0.217	0.147
Cl_I	0.851	0.084	0.781
Cl_{II}	0.641	0.105	0.289
O_I	0.36	0.15	0.93
O_{II}	0.23	0.15	0.49

Table 4.

Interatomic distances in $BaCl_2$, 2 H_2O.

No.	Kind	Distance	Radius Sum
a	$Ba - Cl_I$	3.11 Å	3.20 Å
b	$Ba - Cl_I$	3.27 -	”
c	$Ba - Cl_{II}$	3.16 -	”
d	$Ba - Cl_{II}$	3.24 -	”
e	$Ba - O_I$	2.78 -	2.77 A
f	$Ba - O_I$	2.81 -	”
g	$Ba - O_{II}$	2.82 -	”
h	$Ba - O_{II}$	2.80 -	”
i	$O_I - Cl_{II}$	3.18 -	3.19 Å
j	$O_I - Cl_{II}$	3.22 -	”
k	$O_{II} - Cl_{II}$	3.17 -	”
l	$O_{II} - Cl_I$	3.19 -	”
(m	$Ba - Cl_I$	3.38 -	3.20 Å)

Table 5.

Calculated and observed F’s in the hk0 zone of $BaCl_2$, 2 H_2O. CuK_α radiation.

hk	sin θ	F calc.	F obs.	Obs. Int.	hk	sin θ	F calc.	F obs.	Obs. Int.
11	.132	7.6	0	0	25	.414	6.6	0	0
02	.140	$\overline{33.1}$	29.5	m	06	.418	$\overline{25.1}$	15.7	w-m
12	.179	$\overline{2.5}$	0	0	16	.432	9.8	0	0
20	.225	27.4	14.1	w-m	34	.437	$\overline{23.6}$	14.0	w
21	.235	22.3	10.1	w-m	40	.450	0.0	0	0
13	.237	$\overline{21.3}$	21.4	m	41	.455	32.8	12.9	w, w-m
22	.264	$\overline{36.9}$	25.1	m	42	.471	$\overline{22.0}$	12.4	w
04	.278	3.5	0	0	26	.473	$\overline{9.4}$	0	0
14	.300	$\overline{25.2}$	14.1	w	35	.484	18.8	9.1	w
23	.307	$\overline{21.9}$	13.9	w	43	.495	$\overline{24.2}$	12.3	w
31	.345	6.7	0	0	17	.500	$\overline{40.5}$	36.0	m-s
24	.358	32.4	15.7	w-m	44	.528	21.9	11.4	w
32	.365	2.5	0	0	27	.536	$\overline{4.4}$	0	0
15	.366	37.3	25.4	m	36	.537	27.0	8.5	v,w
33	.396	$\overline{20.4}$	10.1	w	08	.556	1.2	0	0

Table 5 (continued).

hk	sin θ	F calc.	F obs.	Obs Int.	hk	sin θ	F calc.	F obs.	Obs. Int.
51	.566	4.2	0	0	211	.797	16.2	0	0
18	.568	5.4	0	0	73	.807	12.2	0	0
45	.569	18.5	9.8	v, w	74	.827	$\overline{19.7}$	0	0
52	.580	27.6	10.5	w	410	.828	$\overline{4.3}$	0	0
37	.592	$\overline{15.3}$	7.1	v	67	.832	$\overline{0.3}$	0	0
53	.600	$\overline{6.1}$	0	0	012	.835	$\overline{15.6}$	9.2	w
28	.600	$\overline{3.8}$	0	0	311	.837	$\overline{16.8}$		
46	.613	8.1	0	0	59	.842	5.6	0	0
54	.627	$\overline{13.5}$	0	0	112	.843	$\overline{12.2}$	0	0
19	.636	23.3	16.5	w-m	75	.854	$\overline{7.1}$	0	0
38	.651	$\overline{19.2}$	8.8	v	212	.865	$\overline{19.0}$	7.7	w
55	.661	2.1	0	0	68	.875	0.5	0	0
47	.663	$\overline{3.2}$	0	0	76	.884	24.4	8.4	w-m
29	.665	$\overline{0.9}$	0	0	411	.888	12.0	5.5	w
60	.676	5.8	0	0	510	.895	17.1	6.1	v
61	.679	31.9	13.4	w-m	80	.900	$\overline{7.5}$	0	0
62	.689	10.2	0	0	312	.900	$\overline{12.1}$	0	0
010	.696	22.1	8.5	v	81	.903	19.1	6.7	w
56	.700	23.8	11.8	w	82	.911	17.2	6.3	w
110	.704	12.2	0	0	113	.911	16.6		
63	.707	$\overline{24.1}$	13.8	w-m.	77	.920	2.9	0	0
39	.711	26.1	13.8		69	.920	$\overline{6.9}$	0	0
48	.716	$\overline{3.4}$	0	0	83	.924	$\overline{20.5}$	5.5	w
64	.730	$\overline{9.3}$	0	0	213	.933	$\overline{8.6}$	0	0
210	.731	11.7	0	0	84	.943	$\overline{18.1}$	*	v
57	.745	$\overline{3.2}$	0	0	412	.948	$\overline{11.3}$	*	v
65	.759	15.0	0	0	511	.950	$\overline{3.3}$	0	0
49	.770	$\overline{10.0}$	0	0	78	.957	$\overline{23.6}$	7.7	w-m
310	.773	19.4	12.4	w	85	.965	9.4	0	0
111	.773	$\overline{18.3}$	12.4	w	313	.965	$\overline{2.2}$	0	0
71	.783	$\overline{4.5}$	0	0	610	.969	5.2	0	0
58	.791	$\overline{37.6}$	18.0	m	014	.974	23.0	7.0	m-s
72	.791	8.1	0	0	114	.980	$\overline{3.6}$	0	0
66	.793	$\overline{8.2}$	0	0					

* visible but not strong enough to show up on photometer curve.

Table 6.

Calculated and observed intensities in a powder diagram of $BaCl_2, 2H_2O$. CoK_α radiation.

hkl	$10^4 \times \sin^2\theta$	θF^2	Obs. Int.	hkl	$10^4 \times \sin^2\theta$	θF^2	Obs. Int.
011	0368	19	0	$\bar{1}41$	2307	38	w
110	0400	24	0	141	2325	3.2	0
020	0442	250	m	132	2328	6.7	0
$\bar{1}01$	0537	226	w	212	2329	37	v
101	0555	50	0	$\bar{2}31$	2390	49	w
$\bar{1}11$	0648	132	0	013	2420	3.5	0
111	0666	316	w	231	2426	0	0
021	0699	56	0	$\bar{1}03$	2571	44	v
120	0731	0.8	0	$\bar{2}22$	2588	2.3	0
$\bar{1}21$	0979	146	v	103	2625	47	v
121	0997	43	0	222	2660	36	v
002	1026	27	0	$\bar{1}13$	2682	49	
012	1137	152	v	310	2712	1.3	0
200	1156	92	0	113	2736	2.9	0
031	1252	21	0	023	2751	0.3	0
210	1267	60	w	042	2796	0	0
130	1284	50		$\bar{3}01$	2831	29.5	v
$\bar{1}12$	1408	0.4	0	301	2885	0.6	0
112	1444	10.2	0	240	2926	31.6	w
022	1468	29	0	$\bar{3}11$	2942	2.1	0
$\bar{2}11$	1506	77	v	311	2996	94	w-m
$\bar{1}31$	1532	108	w-m	$\bar{1}23$	3013	21.3	0
211	1542	21.3	m	051	3022	13.0	0
131	1550	173		320	3043	0.5	0
220	1598	98	w-m	150	3054	44	w-m
$\bar{1}22$	1739	5.0	0	$\bar{1}42$	3067	45	
040	1770	1.5	0	123	3067	47	
122	1775	110	w-m	142	3103	11.4	0
$\bar{2}21$	1837	18	v?	$\bar{2}32$	3141	27	v?
221	1873	5.8	0	$\bar{2}41$	3165	2.0	0
032	2021	118	m-s	241	3201	28	v
041	2027	51		232	3213	12	0
140	2059	31	w	$\bar{3}21$	3273	44	v
$\bar{2}02$	2146	5.7	0	$\bar{1}51$	3302	2.5	0
230	2151	26	v	033	3304	11	v?
202	2218	29	0	151	3320	9	0
$\bar{2}12$	2257	102	v	321	3327	0.6	0
$\bar{1}32$	2292	0	0	$\bar{2}13$	3522	4.3	0

Tabel 6 (continued).

hkl	$10^4 \times \sin^2\theta$	$\theta\ F^2$	Obs. Int.	hkl	$10^4 \times \sin^2\theta$	$\theta\ F^2$	Obs. Int.
$\bar{1}33$	3566	2.3	0	004	4104	3.3	0
330	3596	1.0	0	322	4123	1.8	0
133	3620	1.0	0	$\bar{2}51$	4160	4.8	0
213	3630	0	0	251	4196	9.0	v ?
$\bar{3}12$	3684	1.9	0	014	4215	5.2	
052	3791	10.6	0	061	4239	12.9	
312	3792	1.4	0	160	4271	3.2	0
$\bar{3}31$	3826	3.0	0	$\bar{1}43$	4341	11.9	v
$\bar{2}23$	3853	0	0	340	4371	12.8	
331	3880	4.4	0	143	4395	8.4	
$\bar{2}42$	3916	1.4	0	$\bar{2}33$	4406	3.1	0
250	3921	1.0	0	$\bar{1}14$	4468	6.4	v
223	3961	0.5	0	233	4514	7.7	
060	3982	7.5	v ?	$\bar{1}61$	4519	4.7	
242	3988	8.7		161	4537	0.4	0
$\bar{3}22$	4015	0.9	0	114	4540	0.9	0
$\bar{1}52$	4062	0.4	0	024	4546	23.1	v
043	4079	1.2	0	$\bar{3}32$	4568	2.0	0
152	4098	3.3	0				

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