Physics. - "The Crystal Structure of Red Mercuric Iodide." By J. M. Bijvoet, A. Clafssen and A. Karssen. (Communicated by Prof. W. H. Keesom).
(Communicated at the meeting of January 30, 1926).

1. This investigation was taken up in view of the allotropic behaviour of $\mathrm{HgI}_{2}{ }^{1}$ ).

We intend to investigate at a later date its yellow rhombic modification and the isomorphous $\mathrm{HgBr}_{2}$.

According to Groth ${ }^{2}$ ) red mercuric iodide crystallizes in the ditetragonalbipyramidal class of the tetragonal system, with an axial ratio a $: c=1: 2,008$.

The crystals for our $X$-ray analysis were obtained by slow crystallisation from metyliodide solution and formed dark red quadratic prisms. They possess a very perfect cleavage parallel to the basal plane.

For the rotation diagrams crystals of 1 or 2 mm . diameter were used.
2. Apparatus. This has been described by J. M. Bijvoet and A. Karssen ${ }^{3}$ ). Radius of the camera $2,47 \mathrm{~cm}$. During the exposure the crystals were rotated by clockwork. The exposures lasted about 30 hours with a mean current of 6 milliamps.
3. Determination of the elementary-cell.

The dimensions of the unit cell can be determined by means of rotation diagrams, in which the crystal is rotated about some crystallographic axis. The $X$-ray period ("Identitätsperiode") $I$ along this axis can then be found from the distance of the zone to the equator, according to the formula of PolanyI ${ }^{4}$ ): $I=\frac{n \lambda}{\cos \mu}$. In this formula $n=$ zone-number; $\lambda=$ wavelength and $\mu$ the angle between zone and equator as defined by $\operatorname{tg}(90-\mu)=\frac{l}{R}$ with $R=$ radius of the camera.

Combining these two formulae we get:

$$
I=n \lambda \sqrt{1+\frac{R^{2}}{l^{2}}} .
$$

The following table I gives the measured $X$-ray period of various crystallographic axes, as calculated by the above formula. Each value is an average from several films.

[^0]Table I. X-ray periods.


From the rotation diagrams about [100] and [001] there follows for the dimensions of the unit cell in these directions $6.20 \AA$ and $12.43 \AA$, respectively. This gives an axial ratio agreeing very well with the one determined goniometrically (§ 1).
The [110] period is calculated as $6.20 \mathrm{~V} 2 \AA=8.76 \AA$.
In table I we found $I_{(110)}=4.35 \AA$, hence the [110] period is halved. For the [101] and [111] directions we calculate from the cell dimensions $13,89 \AA$ and $15,22 \AA$ respectively; the $X$-ray periods found (see table I) indicate that these directions are not halved.

The literature gives for the density of red $\mathrm{HgI}_{2} 6.28$ to $6.30{ }^{1}{ }^{1}$ )
${ }^{1}$ ) P. Groth. Chem. Krystall. 1, pag. 218. Van Nest, Z, f. Krystall. 47265 (1910.)

From this the number of molecules per unit cell appears to be 4.
Starting from 4 molecules per cell and the above found cell-dimensions we calculate the density as 6.28 .

This unit cell however is not the smallest one possible. Indeed, the smallest $X$-ray period in the basal plane being equal to $4.38 \AA$, by turning the system of coordinates about the four-fold axis through $45^{\circ}$, a new elementary cell can be assumed with dimensions $12,43 \AA \times(4.38 \AA)^{2}$. This cell contains only two molecules.

The values of $10^{3} \sin ^{2} 9 / 2$ must fulfil a quadratic equation in the Millerian indices, which for the tetragonal system reads:

$$
\sin ^{2} 9 / 2=\frac{\lambda^{2}}{4 a^{2}}\left(h^{2}+k^{2}\right)+\frac{\lambda^{2}}{4 c^{2}} l^{2}
$$

With the above found dimensions of the unit cell, viz.:
$a=4,38 \AA ; c=12,43 \AA$ we get the following formulae for $10^{3} \sin ^{2} \approx / 2$

$$
\begin{aligned}
& 10^{3} \sin ^{2 s} / 2=30,9\left(h^{2}+k^{2}\right)+3,83 l^{2} \text { for } C u K_{\alpha} \\
& 10^{3} \sin ^{29} / 2=68,0\left(h^{2}+k^{2}\right)+8,45 l^{2} \text { for } C r K_{\alpha} .
\end{aligned}
$$

From these equations indices have been assigned to the reflections on the rotation-diagrams about various axes. The excellent agreement between calculated and observed values brings out the correct choice of the unit cell.

The indices referring to the smallest cell ( $h k l$ ) can be deduced from those relating to the crystallographic cell (HKL) by means of the transformation :

$$
h=\frac{1}{2}(H+K), k=\frac{1}{2}(H-K), \quad l=L .
$$

When the observed and calculated values of sine-squares of the rotation diagrams are compared, it appears that the observed values are always 8 to 10 units larger than the calculated ones; this is in good agreement with the corrections to be expected for the thickness of the crystals ( 1 to 2 mm .). The factors in the formulae given above agree well with the powder films corrected for the thickness of the rod.

a. reflection with $\mathrm{CuK} \alpha$

b. reflection with $\mathrm{FeK} \alpha$.

Fig. 1.

Table II．Rotation－diagram about［001］．

| $\lambda=1,539{ }^{\circ} \mathrm{A}$ | Distance in cm ． | 嵌 | $10^{3} \sin ^{2} 9 / 2$ observed | $\begin{aligned} & 10^{3} \sin ^{2} 9 / 2 \\ & \text { calculated } \end{aligned}$ | hkl | $\lambda=1,934{ }^{\circ} \mathrm{A}$ | 免 | 邑 | $\begin{aligned} & 10^{3} \sin ^{2} \mathrm{~g} / 2 \\ & \text { reduced } \\ & \text { to } \mathrm{Cu} K \alpha \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Aequator$l=0$ |  |  |  |  |  |  |  |  |  |
|  | 1.28 | vw | 66 | 62 | 110 |  | 1.63 | W | 66 |
|  | 1.81 | WM | 129 | 124 | 200 |  | 2.35 | w | 133 |
|  | 2.62 | vs | 256 | 248 | 220 |  | 3.41 | vs | 256 |
|  | － | － | － | 495 | 400 |  | 5.45 | S | 504 |
|  | 4.53 | S | 630 | 618 | 420 |  |  |  |  |
| 1st zone$l=1$ |  |  |  |  |  |  |  |  |  |
|  | － | － | － | 35 | 101 |  | 1.25 | Vvw | 41 |
|  | 2.06 | M | 167 | 159 | 211 |  | 2.64 | S | 166 |
|  | 3.46 | WM | 416 | 406 | 321 |  | 4.67 | MS | 415 |
|  | 4.08 | W | 540 | 530 | 411 |  | 5.81 | MS + | 536 |
|  | 5.41 | vW | 789 | 776 | 431 |  |  |  |  |
| 2nd zone$l=2$ |  |  |  |  |  |  |  |  |  |
|  | 1.30 | S | 82 | 77 | 112 |  | 1.69 | S | 84 |
|  | 2.08 | $\mathrm{S}^{-}$ | 178 | ． 170 | 212 |  | 2.70 | S | 178 |
|  | 2.66 | W | 272 | 263 | 222 |  | 3.50 | W | 270 |
|  | 3.02 | WM | 336 | 324 | 312 |  | 3.99 | M | 330 |
|  | 3.51 | MS | 427 | 417 | 322 |  | 4.78 | MS | 423 |
|  | 4.15 | M | 553 | 541 | 412 |  |  |  |  |
|  | 4.31 | vW | 584 | 571 | 332 |  |  |  |  |
|  | 5.53 | M | 800 | 787 | 432 |  |  |  |  |
|  | 5.73 | WM | 830 | 818 | 512 |  |  |  |  |
| 3rd zone$l=3$ |  |  |  |  |  |  |  |  |  |
|  | 2.11 | WM | 196 | 189 | 213 |  |  |  |  |
|  | 3.60 | WM | 447 | 436 | 323 |  |  |  |  |
|  | 4.26 | W | 571 | 560 | 413 |  |  |  |  |
|  | 5.74 | W | 818 | 806 | 433 |  |  |  |  |
| 4th zone $l=4$ |  |  |  |  |  |  |  |  |  |
|  | 1.34 | MS | 128 | 124 | 114 |  |  |  |  |
|  | 3.19 | S | 380 | 370 | 314 |  |  |  |  |
|  | 4.62 | MS | 629 | 617 | 334 |  |  |  |  |
| 5th zone $l=5$ |  |  |  |  |  |  |  |  |  |
|  | 0.77 | W | 131 | 127 | 105 |  |  |  |  |
|  | 2.24 | WM | 258 | 250 | 215 |  |  |  |  |
|  | 3.89 | WM | 502 | 497 | 325 |  |  |  |  |
|  | 4.67 | WM | 627 | 621 | 415 |  |  |  |  |

4. Determination of the positions of the atoms in the unit cell.

In order to determine the positions of the atoms a knowledge of the diffraction intensities from the various planes is necessary.

Table III. Rotation-diagram about [010]; $\lambda=2.286 \AA$

|  | Distance in cm . | Intens. | $\begin{aligned} & 10^{3} \sin ^{2} 9 / 2 \\ & \text { observed } \end{aligned}$ | $\begin{aligned} & 10^{3} \sin ^{2} 9 / 2 \\ & \text { calculated } \end{aligned}$ | $h k l$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Aequator$k=0$ | 2.76 | VS | 281 | $\left.\begin{array}{l} 279 \\ 275 \end{array}\right\}$ | $\left.\begin{array}{l} 105 \\ 200 \end{array}\right\}$ |
|  | 2.94 | S | 314 | $\left.\begin{array}{c} 306 \\ 308 \end{array}\right\}$ | $\left.\begin{array}{l} 006 \\ 202 \end{array}\right\}$ |
|  | 3.31 | W | 386 | 375 | 106 |
|  | 4.14 | $\mathrm{S}^{-}$ | 553 | 543 | 008 |
|  | 4.31 | M | 587 | 577 | 206 |
|  | 4.54 | S- | 632 | 624 | 301 |
|  | 4.67 | S | 657 | 649 | 302 |
|  | 4.89 | $\mathrm{S}^{-}$ | 699 | $\left.\begin{array}{l} 689 \\ 689 \end{array}\right\}$ | $\left.\begin{array}{l}207) \\ 303\end{array}\right\}$ |
|  | 5.64 | vs | 827 | 815 | 208 |
| 1st zone$k=1 .$ | 1.68 | W | 170 | 169 | 112 |
|  | 2.51 | M | 278 | 272 | 114 |
|  | 3.04 | S | 360 | $\left.\begin{array}{l} 348 \\ 352 \end{array}\right\}$ | $\left.\begin{array}{l} 115 \\ 211 \end{array}\right\}$ |
|  | 3.18 | S | 381 | $\left.\begin{array}{l} 373) \\ 375 \end{array}\right)$ | $\left.\begin{array}{l}016 \\ 212\end{array}\right\}$ |
|  | 3.44 | M | 424 | 418 | 213 |
|  | 3.82 | W | 490 | 478) <br> 488) | $\left.\begin{array}{l} 214 \\ 017 \end{array}\right\}$ |
|  | 4.25 | $\mathrm{W}^{+}$ | 564 | $\begin{aligned} & 550 \\ & 554 \end{aligned}$ | $\left.\begin{array}{l}117 \\ 215\end{array}\right\}$ |
|  | 4.81 | M | 656 | 646 | 216 |
|  | 5.26 | MS | 725 | 717 | 312 |
|  | 5.54 | M | 764 | 754 | 217 |
|  | 6.04 | VS | 826 | 818 | 314 |

Table IV. Rotation-diagram about [110]; $\lambda=2.286$ 'A

|  | Distance in cm . | Intens. | $\begin{aligned} & 10^{3} \sin ^{2} 9 / 2 \\ & \text { observed } \end{aligned}$ | $10^{3} \sin ^{2} \mathrm{~s} / 2$ calculated | hkl |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Aequator$h+k=0$ |  |  |  |  |  |
|  | 1.92 | VW | 145 |  |  |
|  |  |  |  | 137) | 170) |
|  | 2.14 | vw | 176 | 170 | $1 \overline{12}$ |
|  | 2.77 | M | 283 | 273 | $1 \overline{14}$ |
|  | 2.92 | MS | 311 | 306 | 006 |
|  |  |  |  | 543) | 008 ) |
|  | 4.15 | VS | 555 | 549 ) | $2 \overline{20}$ ) |
|  | 4.31 | WM | 587 | 581 | $2 \overline{22}$ |
|  | 5.85 | vS | 858 | 852 | $2 \overline{26}$ |
| 1st zone$h+k=1$ |  |  |  |  |  |
|  | 3.11 | S | 358 | 352 | $2 \overline{11}$ |
|  | 3.19 | S | 371 | 369 | 106 |
|  | 3.48 | M | 426 | 418 | $2 \overline{13}$ |
|  | 3.81 | M | 487 | 478 | $2 \overline{14}$ |
|  | 4.20 | W | 561 | 555 | $2 \overline{15}$ |
|  | 4.73 | M | 657 | 647 | $2 \overline{16}$ |
|  | 5.32 | S | 756 | 753 | $2 \overline{17}$ |

A. With a strongly absorbing crystal as $\mathrm{HgI}_{2}$, it is impossible to draw conclusions from intensity-relations on rotation diagrams, without taking account of the influence of absorption. ${ }^{1}$ )

This is obvious from the missing 400 reflection on the Cu -film about [001], which is very strong on the corresponding Fe -film. Now on the Cu -film the angle of deviation $\vartheta$ is smaller than $45^{\circ}\left(10^{3} \sin ^{2} 9 / 2=495\right)$ while on the Fe -film it is greater $\left(10^{3} \sin ^{2} 9 / 2=781\right)$.

In the case of diffraction with Fe -rays, incidence and reflection take place through the same crystal-face (in casu 110); in the case of diffraction with Cu -rays this is impossible (see fig. 1) and the diffracted X-rays must pass through an edge of the crystal. Hence the reflected beam will be nearly totally absorbed except in the very nearest neighbourhood of the crystal-edge. ${ }^{2}$ )
${ }^{1}$ ) A. E. van Arkel, Physica 3 p. 76.
${ }^{2}$ ) Note added during correction. In a recent paper W. L. Bragg and G. B. Brown Proc. Royal Soc. 110, 35 (1926) have drawn attention to this same fact.

For the same reason we should expect the 200 reflection to be absent. It was present however, though very faint. We cannot give an explanation of this fact; ostensibly the prism-sides had not crumbled off.

In the beginning of this investigation we had concluded wrongly that 400 did not reflect, or only faintly. With Cr-rays 400 cannot reflect $(\sin \vartheta>1)$, on the Cu -powder film 400 coincides with other reflections; Table V. Rotation-diagram about [111]; $\lambda=2.286 \AA$

|  | Distance in cm . | Intens. | $\begin{gathered} 10^{3} \sin ^{2} 9 / 2 \\ \text { observed } \end{gathered}$ | $\begin{aligned} & 10^{3} \sin ^{2} \mathrm{~s} / 2 \\ & \text { calculated } \end{aligned}$ | hkl |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{gathered} \text { Aequator } \\ h+k+l=0 \end{gathered}$ |  |  |  |  |  |
|  | 2.17 | MS | 181 | 170 | 112 |
|  | 3.17 | M | 359 | 351 | 2 1 1 |
|  | 3.51 | WM | 425 | 417 | 2 1.3 |
|  | 4.14 | vS | 553 | 546 | $2 \overline{2} 0$ |
|  | 4.89 | W | 699 | 703 | $\overline{3} 3$ |
|  | 5.03 | M | 725 | 715 | $\overline{3} 12$ |
|  | 5.63 | vs | 825 | 816 | 了 $\overline{1} 4$ |
|  | 6.16 | MS | 900 | 895 | $\overline{3} 1$ |
| $\begin{gathered} \text { 1st zone } \\ h+k+l=1 \end{gathered}$ |  |  |  |  |  |
|  | 3.30 | M | 384 | 376 | $\overline{2} 12$ |
|  | 4.68 | w | 659 | 649 | $30 \overline{2}$ |
| $\begin{gathered} \text { 2nd zone } \\ h+k+l=2 \end{gathered}$ |  |  |  |  |  |
|  | 2.02 | MS | 177 | 170 | 1 12 |
|  |  |  |  | ${ }^{273}$ ) | $\overline{1} 14\}$ |
|  | 2.71 | MS | 285 | 274 | 2006 |
|  | 3.17 | M | 362 | 352 | 2 11 |
|  | 3.50 | $\mathrm{w}^{-}$ | 427 | 417 | $\overline{2} 13$ |
|  | 4.22 | W | 565 | 556 | $\overline{2} \overline{1}$ |
|  | 4.34 | W | 586 | 581 | $\overline{2} 2$ |
|  | 5.12 | W | 727 | 716 | $31 \overline{2}$ |
|  | 5.72 | vs | 820 | 817 | $\overline{3} 14$ |
|  | 5.92 | S | 857 | 852 | $\overline{2} \overline{2} 6$ |

hence these photograms could not give any direct information. We had used this absence of 400 for some laborious calculations, which did not lead to any structure. On a photogram taken casually with Fe -radiation we found that 400 did reflect and even strongly.

Table VI. Rotation-diagram about [201]; $\lambda=2.286 \AA$

|  | Distance in cm . | Intens. | $\begin{aligned} & 10^{3} \sin ^{2} 9 / 2 \\ & \text { gbserved } \end{aligned}$ | $10^{3} \sin ^{2} 9 / 2$ calculated | hkl |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Aequator$2 h+l=0$ |  |  |  |  |  |
|  | 2.17 | vs | 180 | 170 | $\overline{1} 12$ |
|  | 3.32 | vs | 388 | 376 | $\overline{122}$ |
|  | 5.04 | S | 726 | 716 | $\overline{1} 32$ |
| 1st zone$2 h+l=1$ |  |  |  |  | $20 \overline{3}$ |
|  | 3.15 | M | 359 | $350\}$ | $12 \overline{1}\}$ |
|  | 3.50 | M | 424 | 418 | $21 \overline{3}$ |
|  | 4.54 | VW | 631 | $\left.\begin{array}{l} 623 \\ 623 \end{array}\right\}$ | $\left.\begin{array}{l} 031 \\ 223 \end{array}\right\}$ |
| 2nd zone$2 h+l=2$ |  |  |  |  |  |
|  | 1.52 | w | 111 | 100 | 012 |
|  | 2.71 | S | 283 | 272 | $\overline{114}$ |
|  | 3.30 | M | 389 | 382 | $21 \overline{2}$ |
|  | 5.72 | vs | 824 | 818 | $31 \overline{4}$ |
|  | 5.98 | S | 859 | 852 | $\overline{2} 26$ |

Rotation-diagrams about [100] were made from Kl, to demonstrate once more on a crystal of known structure that one cannot conclude a structure-factor to be small when the reflection fails on a rotation-diagram. Exposures were made at first on crystals bounded by its ordinary cubefaces, and then with its edges ground off. It was to be expected that in the last case the (110) plane would have to suffer less from absorption. The result is given in table VII.

Table VII. KI Rotation-diagram about [100]; $\lambda=2.286 \AA$

| Plane | Structurefactor | Observed intensities |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  |  | Cube face is reflecting face | Edges ground off |
| 200 | $\mathrm{K}+\mathrm{I}$ | VVS | Boundary face is reflecting face | WM |
| 220 | Item |  | .,Through an edge" | VS |
| 400 | " | VS | Boundary face is reflecting face | WM |
| 420 | " | vs | Not ,through an edge" | VS |
| 440 | " | S | Not ,through an edge" | S |

In interpreting intensities of rotation-diagrams, not only for absorption but for the other influences as well, the factors must be used in their special forms as adapted to this method. So for planes belonging to the zone of the rotation-axis, instead of the powder factor $\frac{1}{\sin ^{29} / 2 \cos 9 / 2}{ }^{1}$, a factor $\frac{1}{\cos 9 / 2}$ must be used for an imbedded crystal. For other planes a factor appears ${ }^{2}$ ) originating from the resolution of the rotation-velocity parallel to the normal on the reflecting plane. We hope to revert to these intensity questions, investigating whether disturbing influences ${ }^{3}$ ) can be limited sufficiently to make rotation-diagrams useful for intensity calculations.
B. Therefore we have based our calculations mainly upon intensitydata from powder-photograms. The exposures were made with Cu - Fe and $C r$-radiation. The intensities were independent of the degree of fineness of the powder. The size of our coarsest powder was $\pm 0,005 \mathrm{~mm}$. Our finest powder, obtained by pouring a methylalcoholic solution into water, was not greater than $0,001 \mathrm{~mm}$.

The exposures with $C u$-radiation were made with a thin $N i$-plate to filter away the $\mathrm{Cu} K_{\beta}$ rays. As contrasted with the Cu - and Fe -films, the $C r$-exposures showed a strong general blackening; they could be used only to determine more accurately the place of the strongest lines. On the Cu -films readings could only be carried out well up to $10^{3} \sin ^{2} 9 / 2= \pm 500$; at greater angles of deviation the lines grew broad and diffuse.

In table VIII the results of the measurements of the powder films are given. The mentioned values of $10^{3} \sin ^{27} / 2$ are averaged over many films and are corrected for the thickness of the rod following GerlachPauli. ${ }^{4}$ ).

In the $4^{\text {th }}$ column the planes are given which may cause the diffraction line; in the $5^{\text {th }}$ column the corresponding calculated values of $10^{3} \sin ^{2} 9 / 2$.

On the $F e$-film, line $n^{0} .11$ is split up into two distinct lines of nearly the same intensity, with values of $10^{3} \sin ^{2} 9 / 2$ (reduced to Cu ) 248 and 252 respectively.
C. Determination of structure.
$\mathrm{HgI}_{2}$ crystallizes tetragonal holohedrally. From table I it follows that the unit-cell is not body-centred. Hence the structure must be one belonging to the space-groups $\left.D_{4 h}^{1} \mp D_{4 h}^{16}\right)$.

[^1]Table VIII. Powderfilm $\mathrm{HgI}_{2}[\mathrm{CuK} \alpha]$.

| No. | Intensity | $\begin{aligned} & 10^{3} \sin ^{2} \mathrm{~F} / 2 \\ & \text { corrected } \end{aligned}$ | Possible planes | $10^{3} \sin ^{29} / 2$ calculated |
| :---: | :---: | :---: | :---: | :---: |
| 1 | MS | 35 | 100; 003; 101 | 31: 34; 35 |
| 2 | S | 47 | 102 | 46 |
| 3 | M ${ }^{+}$ | 67 | 004; 110; 103; 111 | 61; 62; 65: 66 |
| 4 | $\mathrm{M}^{+}$ | 78 | 112 | 77 |
| 5 | vs | 125 | 114; 200; 105; 201 | 123: 124; 126; 128 |
| 6 | W | 141 | 006: 202 | 139: 139 |
| 7 | W ${ }^{+}$ | 161 | 203: 115; 211 | 158: 159: 159 |
| 8 | S | 172 | 106: 212 | 169: 170 |
| 9 | W+ | 191 | 007: 213 | 187: 189 |
| 10 | W | 221 | 214; 107; 205 | 216; 221; 221 |
| 11 116 | M | $252\left\{\begin{array}{l}248 \\ 252\end{array}\right.$ | 008; 220: 117; 215 | 246: 248; 250: 251 |
| 12 | W+ | 264 | 206:222 | 262: 263 |
| 13 | vW | 279 | 108; 300; 301; 223 | 276: 278: 282: 282 |
| 14 | M | 297 | 216:302 | 293: 294 |
| 15 | w | 325 | 312 | 324 |
| 16 | W | 344 | 109: 217: 313: 225 | 341: 343; 343; 344 |
| 17 | MS ${ }^{+}$ | 373 | 208: 314: 119: 305 | 370: 370; 372: 374 |
| 18 | w | 384 | 00 10: 226 | 383; 386 |
| 19 | vW | 407 | 320; 321; 315 | 402; 405; 406 |
| 20 | W ${ }^{+}$ | 419 | 306; 322 | 416: 417 |
| 21 | W ${ }^{+}$ | 447 | 1110; 316 | 445: 447 |
| 22 | vW | 467 | 324: 219:307 | 463: 465 : 466 |

Two molecules of $\mathrm{HgI}_{2}$ must be placed in the unit-cell. Supposing that like atoms are equivalent, the mercury atoms must be placed in two-fold positions and the iodine atoms in four-fold ones.

A first selection of possible cases was based on the intensities of the planes $h k 0$. The c-coordinate of the atoms is immaterial for the formation of their structure-factor. The possible 13 combinations as regards the $a$ and $b$ coordinates, are the following.
two-fold positions: four-fold positions:

| 1 | 0 | $\frac{1}{2}$ | $\frac{1}{2}$ | 0 | 0 | $\frac{1}{2}$ | 0 | $\frac{1}{2}$ | $\frac{1}{2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | 0

The parameter $u$ has a range from $0^{\circ} \rightarrow 180^{\circ}$ in the structures 2,3 , 9,10 and 12 , and a range $0^{\circ} \rightarrow 90^{\circ}$ in $\mathrm{N}^{\circ \mathrm{s}} .6$ and 7. Now for $a$ such a value has to be evaluated, that the course of the intensities of the prismplanes appears. The approximate formula $I=\frac{v S^{2}}{\sin ^{29} / 2}$ is used; in this formula $S=$ structure-factor, $v=$ number of planes-factor. The scattering power of $H g$ and $I$ has been taken as proportional to the number of electrons per ion, 78 and 54 respectively. For these heavy atoms and long waves the ratio of the scattering powers of Hg and $I$ may be taken as approximately independent of $\vartheta$ (see 4 d ).

The estimated intensities of the prism-planes are given in table IX.
These intensities have been derived from powder films and rotationdiagrams. On the powder films lines representing 210 and 310 were missing (See table VIII). About lines 5, 7 and 9 (table IX) nothing can be concluded from the powder-films; in their place lines have been observed which may be due to other reflections. The failure of these lines has been deduced from their non-observed intensity on rotation-diagrams (table I), in which the reflection did not pass through an edge. These reflections have been printed in fat type in table X. Column 2 gives the values of $9 / 2$ for these reflections (which have nowhere been observed); column 5 gives the angle $\varphi$ between reflecting plane and bounding plane. When $9 / 2>\varphi$, the reflection does not pass through an edge and consequently should have been observed. The intensities of lines 1, 2 and 4 are obtained principally from rotation-diagrams about [001] (table I); lines 1 and 4 are reflections from the bounding plane, so that their relative intensities may be obtained safely from rotation-diagrams. Line 2 observed as faint, passes through an edge; hence it must be strong.

Table IX.

| 1 | 110 | VW |
| :---: | :---: | :---: |
| 2 | 200 | $\pm \mathrm{S}$ |
| 3 | 210 | - |
| 4 | 220 | $\pm \mathrm{S}$ |
| 5 | 300 | - |
| 6 | 310 | - |
| 7 | 320 | - |
| 8 | 400 | Present |
| 9 | 330 | - |
| 10 | 420 | Present |

Table X.

| Indices | \%/2 |  |  | $\varphi$ |
| :---: | :---: | :---: | :---: | :---: |
|  | CuK | FeK | CrK |  |
| 210 | $23^{\circ}$ | $29^{\circ}$ | $36^{\circ}$ | $18^{\circ}$ |
| 300 | 32 | 41 | 51 | 45 |
| 310 | 34 | 45 | 56 | 26 |
| 320 | 39 | 53 | 71 | 11 |
| 330 | 48 | 70 | - | 0 |

With table IX the possible cases $1-13$ have been examined with the following result:

1. This case is not possible as planes with $h$ and $k$ odd would have a structure-factor $=2 \mathrm{Hg}+4 \mathrm{I}$.
2. With the intensity ratio of 310 and 400 only $u<30^{\circ}$ and $u>150^{\circ}$ is consistent. This case is derived from $D_{4 h}^{1}$, in which 4 I-atoms have the same c-coordinate; hence their mutual distance should be smaller than $0.8 \AA$. This must be considered as impossible, as, according to BragG ${ }^{1}$ ) the atomic radius of $I$ is equal to $1.40^{\circ} \AA$.
3. To be rejected on the intensity ratio of $110,200,210$, and 310 .
4. Cannot be rejected.
5. This gives $\mathrm{S}_{200}=2 \mathrm{Hg}-4 \mathrm{I}$, which is too small.
6. From the intensities 310 and 400 follows $u<30^{\circ}$ and $u>150^{\circ}$. This case is derived from $D_{4 h}^{14}$, in which only 0 and $\frac{1}{2}$ figure in the c-coordinates. To be rejected because of the relative intensities of 102 and 104,300 and 302,210 and 212 etc.
7. To be rejected from the intensities of 110 and 200.
8. 300 is calculated too strong.
9. To be rejected from the intensities of 110 and 200.
10. To be rejected from the intensities of 110,200 and 300.
11. Same as 1.
12. Impossible on account of the intensities of 110,200 and 210.
13. Impossible because all structure-factors are equal to $2 \mathrm{Hg}+4 \mathrm{I}$. Finally only the fourth case remains, which is found to be derived from the following two structures:

| I $H g: 0 \frac{1}{2} u$ | $\frac{1}{2} 0 \bar{u} ; I: 00 v$ | $00 \bar{v}$ | $\frac{1}{2} \frac{1}{2} v$ | $\frac{1}{2} \frac{1}{8} \overline{v,}$ | $D_{4 h}^{7}$ |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| II | $00 \frac{1}{2}$ | $\frac{1}{2} \frac{1}{2} 0 ;$ | $0 \frac{1}{2} v$ | $0 \frac{1}{2} v+\frac{1}{2}$ | $\frac{1}{2} 0 \bar{v}$ | $\frac{1}{2} 0 \frac{1}{2}-v$, | $D_{4 h}^{15}$. |

[^2](In II the $b$-axis is shifted ${ }^{1 / 2}$ with respect to case 4) ${ }^{1}$ ).
I. Here the structure-factor reads:
$$
S=H g\left\{(-1)^{k} e^{2 \pi i l u}+(-1)^{h} e^{-2 \pi i l u}\right\}+2 I\left\{1+(-1)^{h+k}\right\} \cos 2 \pi l v .
$$

Now all possible structure-factors can be divided into three groups, viz.:

$$
\begin{aligned}
& \text { for the planes pil: } S_{p i l}=H g \sin 2 \pi u l \\
& \begin{array}{lll}
\prime \quad " \quad \text { " } \quad \text { " } \quad \text { " }: S_{p p l}=H g \cos 2 \pi u l+2 I \cos 2 \pi v l \\
, \quad \text { iil: } S_{i i l}=H g \cos 2 \pi u l-2 I \cos 2 \pi v l .
\end{array}
\end{aligned}
$$

Here $i$ represents an odd index; $p$ an even one.
If the reflections observed on the rotation-diagrams are arranged in these groups, a dependance of their intensities on $l$ only should appear in each group (apart of course from the influence of absorption etc.).

Now this happens to be the case in all planes viz.:

$$
\begin{array}{ll}
p i 2 \text { rather strong } & p i 4 \text { missing } \\
p p 2 \text { missing or very faint } & p p 4 \text { missing } \\
i i 2 \text { rather strong } & i i 4 \text { very strong. }
\end{array}
$$

It is not difficult to enclose $u$ and $v$ between rather narrow limits with the help of these data and the fact that 102 is a strong line on the powder film, while 104 fails.

Further calculations, which are omitted to save space, show however that no values of $u$ and $v$ can be found giving reasonable agreement with the observed powder-intensities.
II. This structure is identical with the somewhat simpler form:

$$
H g: 000 \frac{1}{2} \frac{1}{2} \frac{1}{2} ; \quad I: 0 \frac{1}{2} v \quad 0 \frac{1}{2} v+\frac{1}{2} \quad \frac{1}{2} 0 \bar{v} \quad \frac{1}{2} 0 \frac{1}{2}-v .
$$

Here too, just as in $A$, only the c-coordinate contains the parameter and the same splitting up of the structure-factor into three groups can be carried out:

$$
\begin{aligned}
& S_{p i l}=H g\left\{1-(-1)^{l}\right\}+2 i I\left\{1+(-1)^{l}\right\} \sin 2 \pi v l \\
& S_{p p l}=H g\left\{1+(-1)^{l}\right\}+2 I\left\{1+(-1)^{l}\right\} \cos 2 \pi v l \\
& S_{i i l}=H g\left\{1+(-1)^{l}\right\}-2 I\left\{1+(-1)^{l}\right\} \cos 2 \pi v l .
\end{aligned}
$$

According to these formulae the structure-factors of all planes $p p i$ and $i i i$ are zero. Indeed, all these planes are absent on the rotationdiagrams.

Referring to the table above we find the following conditions:

$$
\begin{array}{ll}
S_{p i 2}=2 I \sin 2 v, \text { moderate } & S_{p i 4}=2 I \sin 4 v, \text { small } \\
S_{p p 2}=H g+2 I \cos 2 v, \text { small } & S_{p p 4}=H g+2 I \cos 4 v, \text { small } \\
S_{i i 2}=H g-2 I \cos v, \text { moderate } & S_{i i 4}=H g-2 I \cos 4 v, \text { large. }
\end{array}
$$

From the intensities of 102 and 104 on the powder-film, strong and not observed respectively, it follows that the intensity of 102 must be rather smaller than $104 \beta$. Hence we may require $I_{104}<\frac{1}{5} I_{102}$. From this

[^3]inequality it follows that $\sin 2 v>1.5 \sin 4 v$ and hence in the range of $v$ to be considered: $35^{\circ}<v<55^{\circ}$. For different values of $v$ between these limits, the intensities of the powder film were calculated. The value $v=50^{\circ}$ proved to agree very well with the observed intensities, as will be seen from table XI. The intensities, as given in the third column, are calculated from $I=\frac{\nu S^{2}}{\sin ^{2} 9 / 2} \frac{1+\cos ^{2} \vartheta}{\cos 9 / 2}$.

In $S$ we have taken $\mathrm{Hg}=2,9$ and $\mathrm{I}=2$, which agrees with the ratio of the number of electrons in $\stackrel{+}{\mathrm{H}} \stackrel{+}{-}$ and $-\overline{\mathrm{I}}$-ons. $v$ is the number-of-plane-factor which equals 16 for planes $h k l ; 2$ for $00 l ; 4$ for $h 00$ and $h h 0$; and 8 for $h k 0, h 0 l$ and $h h l$.

The first column of table XI gives all possible combinations of indices, only the planes of the form $i i i$ and $p p i$ are omitted, their structure

Table XI. Powderfilm red $\mathrm{HgI}_{2} \mathrm{CuK} \alpha$.

| Indices | Intens. observed | Intens. calculated | Indices | Intens. observed | Intens. calculated | Indices | Intens. observed | Intens. calculated |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\left.\begin{array}{l}100 \\ 101\end{array}\right\}$ | MS | $\underbrace{0}_{3.7} 3.7$ | $\left.\begin{array}{l} 214 \\ 107 \end{array}\right\}$ | W | $\left(\begin{array}{l} 0.2 \\ 0.5 \end{array}\right\} 0.7$ | $\begin{aligned} & 208 \\ & 314 \end{aligned}$ | MS ${ }^{+}$ | $\left.\begin{array}{l} 1.1 \\ 2.6 \end{array}\right\}$ |
| 102 | S | 4.8 | 008 ) |  | 0.4 | 305 ) |  | 0.2 |
| $\left.\begin{array}{l}004 \\ 110\end{array}\right)$ |  | $\left.\left.\right\|_{0,1} ^{0}\right\}_{1,9}$ | $\left.\begin{array}{l}220 \\ 215\end{array}\right\}$ | $\left.\begin{array}{c} W \\ W \end{array}\right\}$ | $\left.\begin{array}{l} 1.1 \\ 0.8 \end{array}\right\} 2.3$ | 0010 | W | $0$ |
| 110 | $\mathrm{M}^{+}$ | 0.11 .9 | 215 |  | $0.8)$ | 226 |  | $0.7)$ |
| 103 ) |  | 1.8 | 206 ) | $\mathrm{W}^{+}$ | $\left.{ }^{1.0}\right\} 1.2$ | $320$ | VW | $0\}_{0.5}$ |
| 112 | $\mathbf{M}^{+}$ | 2.4 | $222)$ |  | $0.2$ | $321)$ |  | $0.5)$ |
| 104 | - | 0.27 | 108 ) |  | $0.3)$ | 1010 | - | 0.1 |
| $\left.\begin{array}{l}114 \\ 200\end{array}\right)$ |  | $\left.l_{06}^{4.9}\right\}_{8}$ | $300$ | VW | $\left.\begin{array}{l} 0 \\ 0.3 \end{array}\right\}^{0.6}$ | $\left.\begin{array}{l} 306 \\ 322 \end{array}\right\}$ | W+ | $\left.\begin{array}{l}0.3 \\ 0.8\end{array}\right\} 1.1$ |
|  | VS | 2.688 .4 | 301 ) |  | 0.3 | 322 |  | 0.8) |
| 105 |  | 0.9 ) | 216 ) |  | $\left.0^{0.9}\right)_{1.5}$ | 323 | - | 0.4 |
| 006 , | W | $0.55\}_{1.0}$ | 302 ) | M | $\left.0_{0.6}\right\}^{1.5}$ | 1110 ) | W+ | ${ }^{0.9}$ ) 1.0 |
| 202 | W | $0.45{ }^{1.0}$ | 118 | - | 0 | 316 | W | $0.1)^{1.0}$ |
| 210 | - | 0 | 224 | - | 0.03 | $324)$ |  | $0.1)$ |
| 211 | $\mathrm{W}^{+}$ | 1.3 | 310 | - | 0.03 | 219 | VW | $0.4 \bigcirc 0.7$ |
| 106 | S | $0.9\}_{3.2}$ | 303 | - | 0.3 | 307 ) |  | 0.2 |
| 212 | S | $2.3)^{3.2}$ | 312 | W | 0.9 |  |  |  |
| 204 | - | 0.03 | 304 | - | 0.06 |  |  |  |
| 213 | $\mathrm{W}^{+}$ | 1.1 | 109 ) | W | ${ }^{0.3} 3_{0.8}$ |  |  |  |
| 116 | - | 0.06 | 217 ) |  | 0.5) |  |  |  |

factor being identically equal to zero and none of these reflections having been observed.
D. Influence of the dependance of the scattering power on the angle of deviation.

In calculating the above intensities, the influence of heat-motion, the absorption in the rod and the dependance of scattering power on $\vartheta$ are neglected. Hence only intensity-ratio's of lines lying not too far apart may be compared. We tested whether, taking into account this dependance, anything is changed in the intensity-ratio's given in table XI.

An approximate idea of this dependance could be obtained from a paper by Hartree ${ }^{1}$ ). In our case the ratio of the scattering powers appears to be sufficiently constant to neglect its change, comparing only lines not too far apart. This now is required because of the neglect of the absorption in the rod, which cannot be calculated accurately for a heavy powder.
5. Accuracy of the determination of the parameter.

The parameter $v$ can be determined with fairly great accuracy. Indeed $v=53^{\circ}$ is eliminated since for the successive lines $13 \mathrm{v} . \mathrm{w} ., 14 \mathrm{~m}$. and 15 w ., the intensities are calculated as $0,9,1,1$ and 1,5 respectively. On the other hand, with $v=47^{\circ}$ line 18 is calculated weaker than line 19. Hence we may put $v=50^{\circ} \pm 2,5^{\circ}$. We have ascertained that these limits do not alter with permissable changes in the ratio of the scattering powers.

## 6. Discussion of the structure.

Our structure is built up of layers of $\mathrm{HgI}_{2}$, in which each Hg -ion is surrounded nearly tetrahedrally by four I-ions. The distance between a Hg -ion and an adjacent I-ion ( $2,80 \AA$ ) agrees tolerably well with the sum of the atomic radii, respectively amounting to $1,50 \AA$ for Hg in cubic $\mathrm{HgS}^{2}$ ) and $1,40 \mathrm{~A}$ for I in the alkalihalides ${ }^{3}$ ). The distance between successive layers is very large; the distance from an I atom in one layer to the neighbouring Hg -ion in the next layer amounting to $4,98 \AA$.

Apart from the fact that the Hg -ions are not surrounded exactly tetrahedrally by I-ions, the structure changes into the fluorspar-type by compressing the layers in the direction of the c-axis. This is shown on the plate, in which A represents the cell described above containing two molecules, B the crystallographic cell having the basal-diagonal of A for side and hence containing 4 molecules; $C$ the fluorsparstructure obtained by compressing the layers.

[^4]As regards the I-ions, the dimensions of this structure agree remarkably well with those found in $\mathrm{SnI}_{4}{ }^{1}$ ) and in $\mathrm{CdI}_{2}{ }^{2}$ ). In these structures also

the shortest distance in one layer between an I-ion and the adjacent positive ion is in agreement with BraGG's values for the atomic radii; the distance between two I-ons in successive layers is equal to $4,18 \AA$ in case of $\mathrm{HgI}_{2}$, while it amounts to $4,21 \AA$ in both $\mathrm{SnI}_{4}$ and $\mathrm{CdI}_{2}$.
According to HUND ${ }^{3}$ ) these layer-structures should be ascribed probably to the great extent to which the ions can be polarized; in our case it must be the I-ion, for which this has been found already in quite another way ${ }^{4}$ ). Under the influence of the adjacent Hg -ions the I-ion will behave as a doublet, pointing with its positive charge to the next layer. So with large polarisibility the layer-structure should be the stable one, having less energy than the more compact, but unpolarised fluorspar-type. This is in analogy with the calculated case that amongst the rod-models of the water-molecule the compact symmetrical model should be stable with small polarisibility, whereas an asymmetrical model should be stable in the opposite case ${ }^{5}$ ).
The formation of layers in this structure easily accounts for the perfect basal cleavage.

According to Groth ${ }^{6}$ ) $\mathrm{HgI}_{2}$ crystals crystallised from acetone,

[^5]showed bi-axial birefringence and lamellar-structure with mutually perpendicular basal-directions. In connection with Mallard's hypothesis that higher-symmetric crystals should be considered as polysynthetic twins of lower-symmetric lamels ${ }^{1}$ ), it is obvious to suppose the elementary cell of $\mathrm{HgI}_{2}$ to be rhombic and the crystal structure pseudotetragonal. During our X-ray investigation of crystals crystallised from methyliodide no indication of this supposed pseudo-tetragonality was found. The cell dimensions at least can differ only very little from those given above. We intend to investigate these anomalous crystals.

## 7. Summary,

Red tetragonal holohedral $\mathrm{HgI}_{2}$ has been investigated with X-rays by the rotating-crystal-and the powder method. Photograms were made with copper-, iron-, and chromium radiation. The cell dimensions are $\alpha=4,38 \AA$, $c=12.43 \AA$, with 2 molecules to the unit-cell. The density is calculated as 6,28 in good agreement with the values given in the literature 6,28 to 6,30 .

Amongst all possible holohedral space-groups only $\mathrm{D}_{4 H}^{15}$ fits the observed intensities. The atomic positions are:

$$
\begin{array}{rl}
H g & : 000 \\
\quad \frac{1}{2} \frac{1}{2} \frac{1}{2} \\
I: 0 \frac{1}{2} v & 0 \frac{1}{2} v+\frac{1}{2} \quad \frac{1}{2} 0 \bar{v} \quad \frac{1}{2} 0 \frac{1}{2}-v \quad \text { with } v=\frac{50 \pm 2,5}{360} .
\end{array}
$$

The influence of the dependance of the scattering power on the angle of deviation has been considered. Table XI gives the observed and calculated.intensities; the agreement is very good.

On the plate $A$ gives the above structure, $B$ the crystallographic cell containing 4 molecules. The Hg -ions are arranged in a body-centred lattice; each Hg -ion is surrounded nearly tetrahedrally by four I-ions. The structure can be changed into the fluorspar-structure by compressing the layers in the direction of the c-axis. (Plate: $B \rightarrow C$ ). In the alkaliiodides the negative I -ion is surrounded evenly all-round by positive ions. In $\mathrm{HgI}_{2}$ however among the four Hg -ions surrounding each I-ion, two are lying at a distance of $2,80 \AA$, agreeing with the sum of the atomic radii, while the other two are at the much greater distance of $4,98 \AA$. The shortest distance between two I-ions in successive layers ( $=4,18 \AA$ ) agrees remarkably well with the same distance in $\mathrm{SnI}_{4}$ and $\mathrm{CdI}_{2}$ (in both $4,21 \AA$ ).

By the arrangement in layers the excellent basal cleavage is readily explained. The stability of the open marshalling may be explained, according to HUND, by taking into account the polarisation of the I-ion.

In interpreting our photograms the structure was assumed to be holohedral. Complete agreement between observation and calculation being obtained, no indication was found of a supposed pseudo-tetragonality of the structure.

[^6]The smallness of the structure-factor of a plane may be deduced from the absence of the reflection on rotation-diagrams, only when the reflection does not pass "through an edge".

A considerable amount of the experimental work in this investigation has been done with great ability by our amanuensis A. Kreuger.

We are indebted to Prof. Smits for his kind interest.

> Lab. of General and Inorganic Chemistry of the University.

Amsterdam, January 25th 1926.

Note added June $2^{\text {nd }}$.
In the Physical Laboratory of the University Manchester one of us (A. C.) made some measurements on $\mathrm{HgI}_{2}$ with the $X$-ray spectrometer, mainly to determine more accurately the dimensions of the unit cell. These were found to be: $a=4.357 \AA$; $c=12.36 \AA$, accurate to about $0.1 \%$ and fully agreeing with recent data of Havighurst (Am. J. Science 10, 556 (1925) : $a=4.356 \AA$; $c=12.34 \AA$ ), which reached us in the mean-time.

The intensity of reflexion of $\mathrm{MoK} x$-rays from $\mid(110)$ and ( 001 ) planes is given below.
As only small crystals were available only qualitative measurements were made.

|  | $\sin \approx / 2$ | Intens. |  | $\sin \mathscr{F} / 2$ | Intens. |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 110 | 0.11 | vvw | 002 | 0.06 | m |
| 220 | 0.23 | vs | 004 | 0.12 | - |
| 330 | 0.34 | - | 006 | 0.17 | $\mathrm{~s}-$ |
| 440 | 0.46 | vw | 008 | 0.23 | s |
|  |  |  | 0010 | 0.29 | - |
|  |  |  | 0012 | 0.35 | - |
|  |  |  | 0014 | 0.40 | w |

Especially the intensities of the (001) reflexions confirm fully the above structure.
The powder-intensities given by Havighurst agree well with ours. He made no attempt to locate the atoms.


[^0]:    ${ }^{1}$ ) A. Smits, The Theory of Allotropy. London, 1922.
    ${ }^{2}$ ) P. Groth, Chemische Krystallographie I, pag. 218.
    ${ }^{3}$ ) J. M. Bijvoet-A. Karssen. Rec. Trav. Chim. 42, 589 (1923), 43, 680 (1924).
    ${ }^{4}$ ) M. Polanyi, Zeitschr. f. Phys. 7, 170 (1921). 9, 123 (1922). 10, 44 (1922).

[^1]:    ${ }^{1}$ ) In the literature this powder-formula is found used for rotation-diagrams i.a. O. Hassel, Z. f. Kristallographie 61, 92 (1924), pag. 98.
    ${ }^{2}$ ) H. Ott, Z. f. Physik., 22, 201 (1924), pg. 212.
    ${ }^{3}$ ) H. Отt. l. c. pg. 202.
    ${ }^{4}$ ) W. Gerlach and O. Pauli. Z. f. Physik. 7, 117 (1921).
    ${ }^{5}$ ) P. Niggli. Geom. Kristalogr. d. Diskont. pg. 129.
    R. W. G. Wyckoff. The analytical expression of the theory of space groups.

[^2]:    ${ }^{1}$ ) W. L. Bragg. Phil. Mag. 40, 169 (1920).

[^3]:    ${ }^{1}$ ) Notation see Wijckoff l.c.

[^4]:    ${ }^{1}$ ) D. R. Hartree. Phil. Mag. 50, 289 (1925).
    ${ }^{2}$ ) N. H. Kolkmeyer. J. M. Bijvoet en A. Karssen. Rec. trav. Chim. 43, 677 (1924).
    ${ }^{3}$ ) W. L. Bragg. Phil. Mag. 40, 169 (1920).

[^5]:    ${ }^{1}$ ) R. G. Dickinson. Journ. Am. Chem. Soc. 45, 958 (1923).
    ${ }^{2}$ ) R. H. Bozorth. Journ. Am. Chem. Soc. 44, 2232 (1922).
    ${ }^{3}$ ) F. Hund. Phys. Z. 26, 683 (1925).
    ${ }^{4}$ ) M. Born en W. Heisenberg. Z. f. Physik. 23, 388 (1924).
    5) W. Heisenberg. Z. f. Physik 26, 196 (1924), F. Hund id. 31, 81 (1925).
    ${ }^{6}$ ) P. Groth. Chemische kristallographie I, pg. 218.

[^6]:    ${ }^{1}$ ) F. M. JaEGER. Inleiding tot de studie der kristalkunde, pg. 202.

