

Physics. — “*Research by means of Röntgen-Rays on the Structure of the Crystals of Lithium and some of its Compounds with Light Elements. II. Lithium-Hydride*”. By J. M. BIJVOET and A. KARSSSEN. (Communicated by Prof. P. ZEEMAN).

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1. *Introduction.* The investigation with X-rays on the structure of lithium-hydride was taken up in connection with the analogy drawn by MOERS¹⁾ between lithium hydride and the heteropolar alkali halogenides.

2. *Röntgenograms.* The photographs were made as described in our preceding paper²⁾. The difficulty presented itself that after the exposures the hydride-content had been reduced by 15 or 20 percents of weight. The parasitical lines were eliminated: by comparing the photographs of samples of decreasing hydride-content (the place of the LiH-lines appeared to be independent of the degree of decay, hence no formation of mixed crystals); by photographing a coarse crystallized, non-rotated sample, appearing the interference lines of LiH markedly distinguished by dots of greater intensity; by checking up the parasitical lines by those of LiOH).

3. *Calculation.* The table contains for LiH the values of $10^3 \sin^2 \frac{\theta}{2}$ for the centres of the α -lines. As appears from the occurrence of a factor $77,5 \pm 0,5$ LiH is regular, and the side of the elementary cell $a = 4,10 \cdot 10^{-8}$ cm. From this common factor the number of particles per elementary cell, n is calculated to be 4.30, with the aid of the density according to MOERS, mol. weight, constant of AVOGADRO, and wavelength $Cr_{K\alpha}$ (resp. 0,816; 7,94; $0,6062 \cdot 10^{14}$ and $2,284 \cdot 10^{-8}$). This points to $n = 4$, which is in agreement with the supposed NaCl structure together with the absence of the planes of mixed indices.

¹⁾ MOERS, Z. f. allg. u. anorg. Chem. **113**, 179, (1920).

NERNST, Z. f. Elektrochemie **26**, 323 and 493 (1920).

²⁾ BIJVOET and KARSSSEN. These Proceedings Vol. XXIII, p. 1365.

Putting $n=4$ the said common factor determines the density at $0,76 \pm 0,01^1$). In absence of all further crystallographical data we have confined ourselves to the question whether sticking to a NaCl or ZnS structure an electron grouping could be found, according to the intensities of the reflections found.

The table gives the observed and calculated intensities. Only those factors which bring about an abrupt change in the intensity as function of Σ/h^2 , have been taken into account, viz. the factor of the number of planes and the structure factor, in which the influence of the configuration of the electrons too has been accounted for. For this were tested some approximative suppositions. We have considered the possibility that the valency-electron remains near its mother-nucleus (atomic lattice); that the Li has lost its valency-electron to the hydrogen (ion lattice)²); that binding of Li and H takes place by means of rings of electrons revolving round the connecting line in planes normal to the non intersecting trigonal axes halfway the Li and H nuclei (binding circles; passing along a trigonal axis two-electron-rings may be imagined between Li and H: molecular lattice, case A; or one-electron-rings between Li and H as well as between H and Li, case B).

As to the orbits of the electrons it has been assumed: 1. that the electrons are so near to their nucleus that they may be supposed to lie in one point (points; reflecting power proportional to the number of electrons); 2. that the connecting line of nucleus and electron is of a definite length ϱ , and is equally occurring in all orientations throughout the part of the crystal that is cooperating in the interference (spheres; diminishing factor for such an electron

$\frac{\sin 2\pi \frac{\varrho H}{a}}{2\pi \frac{\varrho H}{a}}$, in which $H = \sqrt{\Sigma h^2}$ ³); and 3. that these connecting

lines are in planes normal to the non-intersecting trigonal axes, all the directions equally occurring in those planes (rings: diminishing factor $J_0 \left(2\pi \frac{\varrho H}{a} \sin \gamma \right)$, in which J_0 is the Bessilian-function of the order of magnitude 0 and γ the angle between orbit and lattice plane⁴). In the binding circles also only circular orbits have been

¹) Imiprities have no influence on this value of the densty, as there is no formation of mixed crystals.

²) Also the less probable case Li-H⁺ has been considered.

³) Cf. KOLKMEYER, These Proc. Vol. XXIII N^o. 1, p. 120.

⁴) Cf. COSTER, These Proc. Vol. XXII N^o. 6, p. 536.

Number.	$10^3 \sin^2 \frac{\alpha}{2}$ (observed).	Plane indices.	Observed Intensities	Calculated Intensities.														
				Points.				Spheres ¹⁾ .				Rings ¹⁾ .				Binding-circles. ²⁾		Rings. ³⁾
				NaCl-str.		ZnS-str.		NaCl-str.		ZnS-str.		NaCl-str.		ZnS-str.		NaCl-str.		NaCl-str.
				ions.	atoms.	i.	a.	i.	a.	i.	a.	i.	a.	i.	a.	A.	B.	i.
1	232	<i>III</i>	z	0	32	64	80	7	26	36	52	7	26	37	53	37	32	10
2	312	<i>200</i>	ms	96	96	0	24	40	51	8	18	38	50	9	18	16	16	30
3	616	<i>220</i>	ms	192	192	192	192	36	56	36	56	38	57	38	57	39	39	35
4	853	<i>311</i>	zs	0	96	192	240	94	55	70	64	99	54	71	62	102	96	70
5	934	<i>222</i>	s	128	128	0	32	14	21	31	17	19	56	25	19	34	35	42

¹⁾ In this according to BOHR, Phil. Mag. [VI] 26, 490 (1913).

Radius inner ring Li = 0,20 Å
 „ outer ring Li = 0,65 „
 „ H⁻-ring = 0,55 „
 „ H⁻-ring 0,73 „

²⁾ $\rho = 0,2$ a

³⁾ In this

Radius Li⁺-ring = 0,05 a
 „ H⁻-ring = 0,6 a

considered, and here too relation of phases has been neglected (diminishing factor as under 3).¹⁾

The influence of the heat motion, of which nothing is known for the different electrons, was left out of consideration. The radius of the comparatively small inner ring of Li has always been taken equal to BOHR's initial value²⁾; in all the suppositions mentioned it has been examined what values of the radii of the other orbits made the calculated and observed intensity concordant. Finally the supposition "rings, $\varrho_{\text{H}} = \pm 5/6$ times the radius of a two-quanta ring in a free H^- -ion" appeared to give the best agreement. As a specimen some of the calculated intensities are given i. a. those for BOHR's initial values of ϱ , and in the last column the case $\varrho_{\text{H}} = \pm 0,6a$ and $\varrho_{\text{Li}} = \pm 0,05a$, which is in agreement with the observations.

In how far the factors neglected here, as heat motion, and the occurrence of non-circular orbits, may affect the conclusions drawn here, must at present be left undecided.

4. *Summary.* The Röntgenogram of lithium hydride (method DEBYE-SCHERRER) has been taken with K_{Cr} rays. LiH appears to crystallize regularly with 4 LiH per elementary cell. [Side $a = 4.10 \cdot 10^{-8}$ cm.]. The density is found to be $0,76 \pm 0,01$. On the basis taken for the calculation the following assumptions appeared to be most satisfactory: NaCl-structure with positive Li-ions and negative H-ions; systems of two-electron rings both round Li- and H-nuclei with radii resp. $\pm 0,05a$ and $\pm 0,6a$, the planes of which are normal to non-intersecting trigonal axes.

In conclusion we express our great indebtedness to Prof. SMITS for his valuable help and the great interest he took in our work.

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¹⁾ In COSTER's computation of the binding circles of diamond this has also been introduced, whereas KOLKMEYER bases his calculations on an undisturbed phase relation.

²⁾ BOHR, Phil. Mag. (VI) 26 490 (1913).