

Table II

Intensity of line I	<i>hkl</i>	θ	$\sin^2\theta$	<i>d</i> , Å	<i>a</i> , Å
Medium	410	8°38'	0.0225	2.37	3.35±0.05
Weak	200	12°20'	0.0457	1.66	3.33±0.03
»	210	13°37'	0.0554	1.51	3.38±0.04
»	211	15°02'	0.0673	1.37	3.35±0.05
»	220	17°28'	0.0901	1.18	3.35±0.03
Extremely weak	300	18°45'	0.1033	1.107	3.32±0.02
»	221	20°24'	0.1214	1.021	3.38±0.03
»	311	21°16'	0.1316	0.981	3.39±0.03
Very weak	222				
				Mean value	3.36±0.04

a is the lattice parameter of the new phase at atmospheric pressure.

The indexing showed that the high-pressure phase has a structure of the CsCl type. The average lattice parameter is $a_0 = 3.36 \pm 0.04$ Å; the density of the new phase is $\rho = 2.535$ g/cc; the density of the original phase is, according to the x-ray data, $\rho_0 = 2.165$ g/cc. The change of volume occurring during this transformation is $\Delta V = 14.2\%$ per mole.

If we follow the conclusions of Goldschmidt^[14] that a transition accompanied by a change of coordination number from 6 to 8 leads to an increase of 3% in the distance between the differing ions, the predicted lattice parameter of the new phase of NaCl is 3.35 Å. This value is in good agreement with that found. A possible value for the lattice parameter of the new phase can also be obtained from the more general consideration that in a similar transformation the distance between nearest neighbors and the density of the substance both increase. If *a* is the lattice parameter of the transformed phase, and *b* that of the original, then from the first condition after the transformation we have $a > b \cdot 3^{-1/2}$ and from the second $a < b \cdot 2^{-2/3}$. It can be assumed, then, that the parameter *a* can be confined between the close limits

$$0.58 b < a < 0.63 b.$$

For $b = 5.64009$ Å, as in NaCl, the parameter *a* for the CsCl type structure should, under normal conditions, obey the relation $3.26 < a < 3.55$.

In Table III are assembled data for a series of salts which are transformed under pressure or temperature from the NaCl type structure to the CsCl type. For all salts except KI ($a = 4.13$ Å), the lattice parameters for the CsCl type structure satisfy well the inequality given above. More plausibly, in the case of KI the results given in the literature^[7] are too high.

We also determined the variation of volume with pressure for the new phase. This variation

Table III

Compound	<i>b</i> , Å (NaCl type)	<i>a</i> , Å (CsCl type)	Limits of possible value
RbCl	6.56	3.82	$3.70 < a < 4.12$
RbI	7.32	4.34	$4.23 < a < 4.60$
KI	6.06	4.13	$3.51 < a < 3.81$
CsCl	7.10	4.20	$4.10 < a < 4.46$
NH ₄ Cl	6.53	3.86	$3.77 < a < 4.11$
NH ₄ Br	6.90	4.05	$3.99 < a < 4.33$
NH ₄ I	7.24	4.37	$4.18 < a < 4.55$

is described by the equation (see Fig. 1)

$$-\Delta V/V_0 = 14.30 \cdot 10^{-2} + 36.0 \cdot 10^{-7} p - 60.0 \cdot 10^{-12} p^2,$$

where V_0 is the volume occupied by one molecule in the NaCl structure.

We also noted traces of the new phase after removing the pressure from the specimen. It might have been supposed that the preservation of the new phase after removing the pressure in the camera was aided by some pressure "locked" in the bore of the cone; however, an estimate of such residual pressure from the displacement of the lines of the original phase gives a value not greater than 600 atm.

A quantitative phase analysis which we made enabled us to evaluate the approximate proportion of the new phase in the specimens. It is known that the intensity of the diffraction rings for NaCl varies linearly with the volume of the substance participating in the scattering. Therefore the intensities of the lines in the x-ray photographs from the mixed specimens were compared with the intensities of the lines from specimens with 100% of the original phase.

The phase analysis showed that the specimen contained on average 2% of the new phase after the pressure was removed.

DISCUSSION OF RESULTS

It can now be affirmed that in table salt pressure causes a polymorphic transition with a