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TEMPERATURES OF THE IMPULSE  
COMPRESSION OF IONIC CRYSTALS

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In [1, 2] a nonparametric calculation of impulse adiabatics of ionic crystals in B1 and B2 phases was given. The relations  $p_H = p_H(V)$  obtained enable the temperature of the impulse compression  $T_H$  to be obtained for the crystals considered in both phases and enable the effect of the B1  $\rightarrow$  B2 phase transition on the  $T_H = T_H(p_H)$  curves to be investigated.

Taking the energy of the thermal vibrations in the form  $C_V T$  with constant heat capacity  $C_V$  and writing the internal energy using the impulse adiabatic equation we obtain the following equation for the temperature of the impulse compression [3]:

$$T_H = \left[ \frac{1}{2} p_H(V)(V_0 - V) + E_0 - E_x(V) \right] / C_V, \quad (1)$$

TABLE 1

Crystal	B1 phase		B2 phase	
	$p_H$ , kbar	$T_H$ , °K	$p_H$ , kbar	$T_H$ , °K
LiF	64	319	548	527
	175	366	941	1490
	335	502	1550	3430
	569	792	2540	7330
	915	1420		
NaF	54	329	199	374
	115	389	352	998
	202	505	582	2 130
	325	788	937	4 150
	501	1340	1503	7 880
NaCl	12	308	108	533
	31	337	171	100
	56	384	263	1 850
	91	473	393	3 140
	136	643	587	5 380
	198	944	886	9 140
282	1520	1370	15 940	
KCl	27	313	56	362
	50	343	99	715
	80	452	163	1 370
	120	627	255	2 400
	176	970	394	4 280
	253	1630	614	7 430
362	2650	979	13 280	
KBr	26	317	51	435
	44	351	89	803
	69	444	142	1 430
	101	614	219	2 460
	145	989	333	3 396
	206	1460	511	7 322

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TABLE 2

Crystal	Calculated for $T =$ $K \cdot p_H$ , kbar	Calculation from the impulses adiabatic		Experi- ment† $p_H$ , kbar
		$p_H$ , kbar	$T_H$ , °K	
LiF	540	920	1400	—
NaF	150	270	700	240
NaCl	63	105	513	300
KCl	27	55	370	20
KBr	240	40	350	17

\* From [5, 9].

† Data for NaF from [10] from impulse measurements, for NaCl from [6] and KCl and KBr from [11] from static measurements at room temperature.

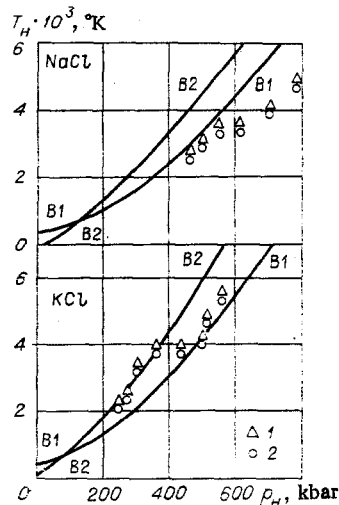


Fig. 1

where  $E_X(V)$  is the energy of the lattice at absolute zero, and  $E_0$  and  $V_0$  are the energy and volume of the free crystal at room temperature. Table 1 shows the results of a calculation using Eq. (1) of the temperatures  $T_H$  for crystals of LiF, NaF, NaCl, KCl, KBr in B1 and B2 phases. To calculate the temperatures for the B1 lattices we used as  $p_H(V)$  and  $E_X(V)$  the functions defined in [1, 2] without including experimental data, while the quantities  $E_0$  and  $V_0$  were found from the energy minimum of  $E_X(V)$ . The temperatures of impulse compression for the B2 lattices were calculated from Eq. (1) in which the values of  $p_H(V)$  and  $E_X(V)$  were taken from [1, 2] for the B2 phase, while the initial characteristics of  $E_0$  and  $V_0$  were related to the B1 phase corresponding to the free crystal.

The results of the calculation of  $T_H$  for NaCl and KCl are shown in the figure, where it can be seen that in the case of NaCl up to 600 kbar there is good agreement between the  $T_H = T_H(p_H)$  curve of the B1 phase and the experimental values of the temperatures measured in [4] (points 1 and 2 are taken from [4]). At a pressure of about 600 kbar the NaCl melts which causes a divergence between the calculated curve and the experimental data, which suffer a sharp discontinuity. Note that for NaCl the B1  $\rightarrow$  B2 phase transition predicted by theory [5] and recorded in static measurements [6] do not appear in experiments on impulse compression [4, 7]. A crystal of KCl at a pressure of  $\sim 20$  kbar suffers a transition to the B2 phase, expressed in the form of a discontinuity in the impulse adiabatic  $p_H = p_H(V)$ . As can be seen from Fig. 1 the experimental points [4], which relate to the dense phase, are very close to the calculated curve of the B2 phase. At a pressure of around 400 kbar KCl melts, producing a discontinuity in the temperature curve and disagreement with the calculation. In the case of a KBr crystal, which suffers a phase transition at a low pressure, the agreement between the calculated curves of the B2 phase and the experimental data [8], relating to the dense phase, is also good. We do not know the experimental values of  $T_H$  for other crystals.

The results obtained were used to estimate the pressures  $p_t$  and the temperatures  $T_t$  of the phase transition. Since at the phase-transition point the pressures and temperatures of both phases are the same, the curves of  $T_H = T_H(p_H)$  of the two phases should intersect, which enables one to estimate the quantities  $p_t$  and  $T_t$ . The results of these estimates for crystals of LiF, NaF, NaCl, KCl, KBr are shown in Table 2, where we also show the transition pressures calculated in [5, 9] at absolute zero, and the experimental values [6, 10, 11]. It follows from a comparison of the second and third columns of Table 2 that the B1  $\rightarrow$  B2 transition pressures increase as the temperature increases. There is good correlation between the values of  $p_t$  calculated from the impulse adiabatics, as calculated in [5, 9], and the values found experimentally in [6, 10, 11].

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