TABLE IV. Pressure derivatives of adiabatic and isothermal elastic constants for NaCl.

T (°K)	$(\partial B^s/\partial P)_T$	$(\partial B^T/\partial P)_T$	$(\partial C_{11}{}^s/\partial P)_T$	$(\partial C_{11}{}^T/\partial P)_T$	$(\partial C_{12}{}^s/\partial P)_T$	$(\partial C_{12}{}^T/\partial P)_T$	$(\partial C/\partial P)_T$
300	5.274	5.369	11.830	11.925	1.997	2.092	0.370
261	5.240	5.324	11.892	11.976	1.914	1.998	0.355
222	5.111	5.180	11.563	11.633	1.859	1.929	0.312
180	4.728	4.822	11.110	11.204	1.536	1.631	0.340

RESULTS

We present our data in a series of tables, Table I–VIII. We have given both the pure adiabatic and the pure isothermal pressure derivatives. The plots of the elastic constants as a function of pressure at $T = 300$°K are given in Figs. 1–4. In Fig. 5, we have plotted the temperature variation of the pressure derivatives along with the data of Bartels and Schuele[2] at 195° and 295°K. The derivatives themselves are good within 5%. The variation, however, is outside the error. All the derivatives decrease very slowly with decreasing temperature and a rather "strange" behavior is exhibited below about 190°K; $\partial C_{11}/\partial P$ and $\partial C_{12}/\partial P$ go down, while $\partial C_{44}/\partial P$ starts going up. Bogardus[3] has reported that

$$[\partial C_{11}/\partial P]_{523°K} < [\partial C_{11}/\partial P]_{300°K}$$

while

$$[\partial C_{44}/\partial P]_{523°K} > [\partial C_{44}/\partial P]_{300°K}.$$

It appears that the variation does not strictly follow the simple quasi-harmonic behavior. In a recent paper Ghafelehbashi et al.[6] also reported a minimum around 200°K in the variation of $[\partial C_{44}/\partial P]$ with temperature for RbCl, for example. At this point we can only say that more work is indeed needed in a wide range of low temperatures. Such an effort is underway in our laboratory.

We have also calculated the mode Grüneisen parameters by using Slater's relation and our pressure-derivative data. The detailed analysis of the computation of macroscopic Grüneisen parameter and its temperature dependence will be dealt with in a future article on that subject covering other alkali halides.

Ruoff[7] has developed an equation of state, based on the bulk modulus variation with pressure of the form

$$B^s = B_0{}^s + B_0{}^{s'}P + B_0{}^{s''}(p^2/2),$$

TABLE V. Grüneisen γ_i for several modes of vibrations using relation $\gamma_i = -\frac{1}{6} + (B^T/2C_i)(\partial C_i/\partial P)_T$, where C_i are the elastic constants and B^T is isothermal bulk modulus.

| Direction of propagation	NaCl					
	γ_L (Longt.)[a]	$\gamma_L{}^b$	γ_{T_1} (shear)[a]	$\gamma_{T_1}{}^b$	γ_{T_2} (shear)[a]	$\gamma_{T_2}{}^b$
			$T=300$°K			
100	2.669	2.62	0.176	0.17	0.176	0.17
110	1.796	1.78	0.176	0.17	3.021	2.91
111	1.455	1.45	1.283	2.20	2.283	2.20
			$T=261$°K			
100	2.672	...	0.167	...	0.167	...
110	1.803	...	0.167	...	3.015	...
111	1.458	...	2.293	...	2.293	...
			$T=222$°K			
100	2.580	...	0.131	...	0.131	...
110	1.753	...	0.131	...	2.860	...
111	1.423	...	2.190	...	2.190	...
			$T=180$°K			
100	2.460	...	0.163	...	0.163	...
110	1.666	...	0.163	...	2.774	...
111	1.342	...	2.146	...	2.146	...

[a] Present work.   [b] Bartels, Ref. 2.
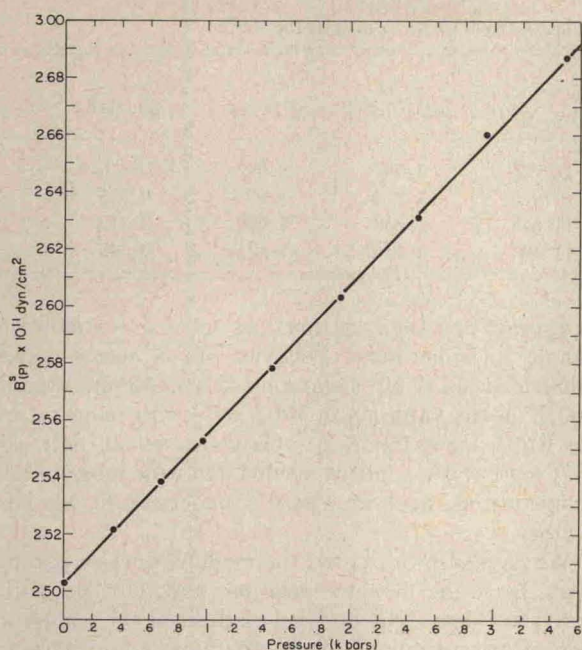
FIG. 1. Variation of the adiabatic elastic constant $C_{11}{}^s$ as function of pressure at $T = 300°$K.

where $B_0{}^s$, $B_0{}^{s\prime}$, and $B_0{}^{s\prime\prime}$ are the zero-pressure bulk modulus and its first and second pressure derivatives respectively. The resultant equation of state is then combined with the Rankine–Hugoniot conservation relations to obtain a Maclurin series for the shock-velocity versus the particle-velocity relationship
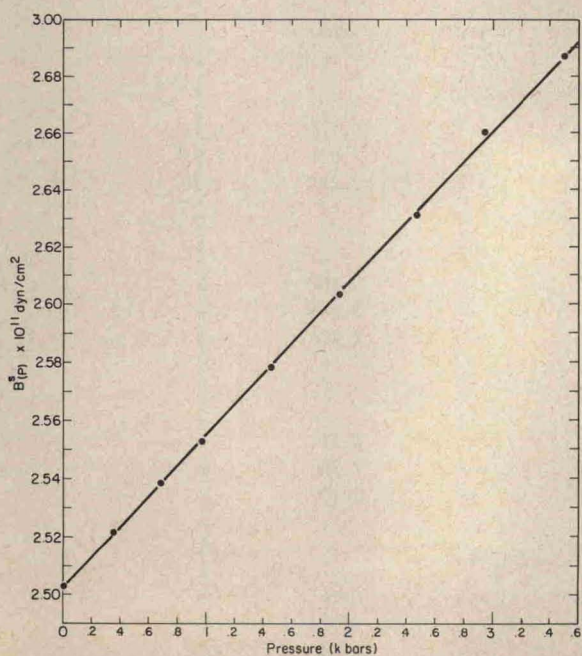
$$U_s = c + s U_p + s' U_p{}^2 + \cdots .$$

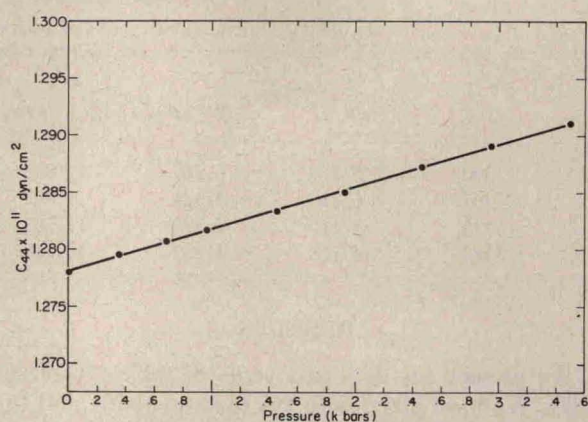FIG. 2. Variation of the adiabatic bulk modulus, (B^s), as function of pressure at $T = 300°$K.

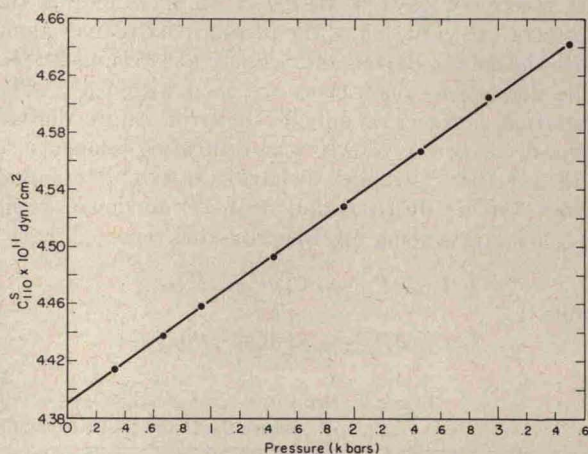FIG. 3. Variation of the elastic constant C_{44} as function of pressure at $T = 300°$K.

FIG. 4. Variation of the adiabatic elastic constant $C_{110}{}^s$ as a function of pressure at $T = 300°$K. $(C_{110}{}^s = C_{11}{}^s + C_{12}{}^s + 2C_{44})/2$.
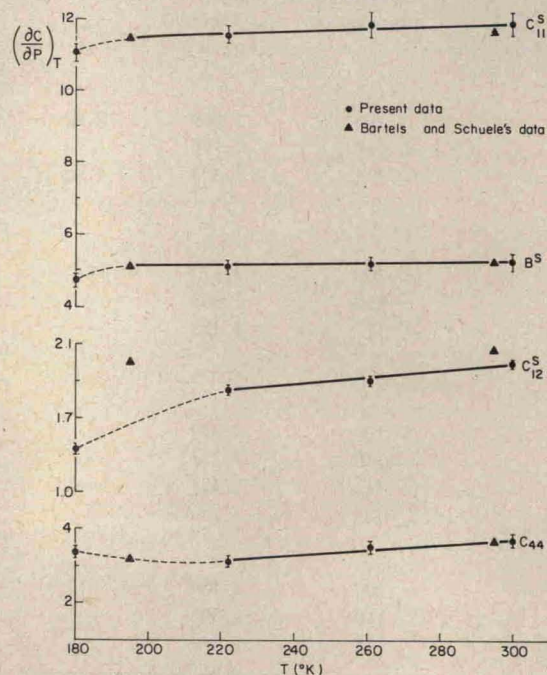

FIG. 5. Temperature variation of $(\partial C_{ij}{}^s / \partial P)_T$.