

pressure. We list the data of *Dobretsov* and *Peresada* in two ways: the average change over the whole pressure range, and the initial slope of their quadratic fit. Some of the discrepancies may arise because of the different range of pressures involved. While none of the pressure derivatives that we measure directly differ from the results of *Bartels* and *Schuele* by more than a few percent, these discrepancies combine to yield a 10% disagreement in  $dK_S/dP$ ; however, our  $dK_S/dP$  is in excellent agreement with that of *Dobretsov* and *Peresada*.

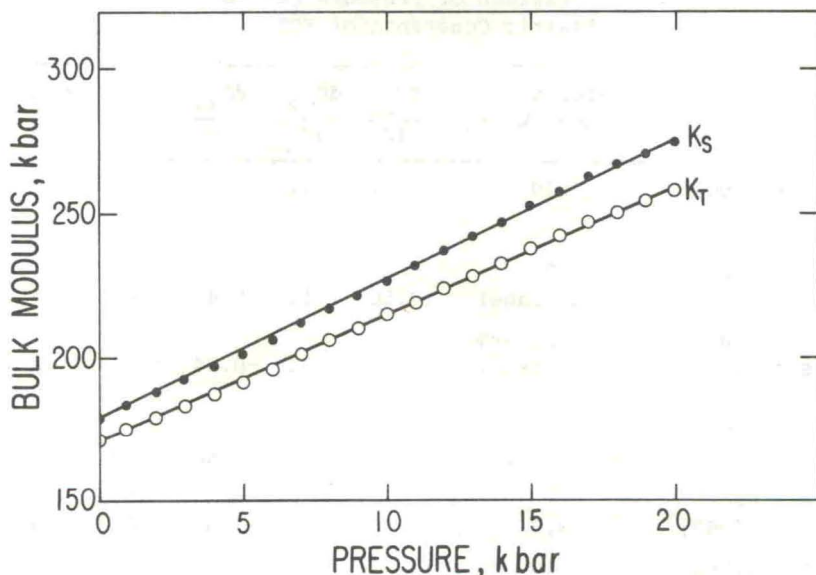


Fig. 4. Variation of adiabatic and isothermal bulk moduli,  $K_S$ ,  $K_T$ , with pressure for KCl single crystal.

There is only a small amount of data from other compounds relating to the problem of the behavior of shear constants at a phase transition. *Reddy* and *Ruoff* [1965] showed that the elastic constants of RbBr are linear right up to the transition pressure at 4.5 kbar. Recent advances in the measurements of velocities in polycrystalline aggregates to pressure on the order of 100 kbar or more [*Voronov* and *Grigor'ev*, 1969; *Morris*, et al., 1976; *Frankel*, *Rich*, and *Homan*, unpublished] are able to provide useful information on the average sound velocities at high pressure. *Voronov* and *Grigor'ev* showed that the average shear velocity in AgCl decreased with pressure prior to the transition, which implies

that at least one of the single-crystal shear moduli ( $C_{44}$ ) decreases toward the transition, but does not provide the much desired measurement of  $\alpha$ . Frankel, et al., report sound velocities in polycrystalline NaCl to 27 GPa, just short of the transition, and they show a slight decrease of  $v_s$  leading up to the transition. Their data appear to be consistent with a model calculation [Demarest, 1972a] that predicted  $C_{44}/K = 0.14$  at the transition.

TABLE 4. Comparison of Pressure Derivatives of Elastic Constants of KCl

	Pressure Range, kbar	$\frac{dC_{11}}{dP}$	$\frac{dC_{12}}{dP}$	$\frac{dC_{44}}{dP}$	$\frac{dC_s}{dP}$	$\frac{dK_s}{dP}$
Present study	20	12.51	0.91	-0.41	5.80	4.78
Wang [1973]	20	-	-	-0.40	-	-
Dobretsov and Peresada [1969]	20 (average)	12.56	1.14	-0.43	5.14	4.81
Dobretsov and Peresada [1969]	linear term of quadratic fit	13.23	0.82	-0.34	5.80	5.12
Drabble and Strathen [1967]	0.004	13.00	1.56	-0.56	5.72	5.37
Bartels and Schuele [1965]	03.3	12.82	1.60	-0.39	5.61	5.34
Lazarus [1949]	10	12.21	1.09	-0.47	5.56	4.80

#### IV. EVALUATION, PREDICTIONS, AND CONCLUSIONS

The Born criterion for a phase transition has often been used to predict a transition at the pressure at which a shear constant vanishes. This is only the upper limit for a transition pressure, however, and any reasonably intelligent method of selecting a pressure somewhere between zero and the Born transition pressure would give more accurate predictions. On the basis of our earlier discussion, we believe that the best prediction of a phase transition which we can base on elastic constant data arises from the assumption that a transition will occur when  $C_t/K$  reaches a critical value  $\alpha$ .

Table 5 displays some selected data relating to the value of  $\alpha$  at a transition. We have grouped compounds with the same crystal structure together, and for each compound we either compute the "measured" value of  $\alpha$  (usually by extrapolating the