

TABLE III

Lattice Vibrations for Alkali Halides<sup>(1)</sup>  $\text{cm}^{-1}$ 

	$\nu_{\text{TO}}$
LiF	307
LiCl	191
LiBr	159
NaF	246
NaCl	164
NaBr	134
NaI	117
KF	190
KCl	141
KBr	113
KI	98
RbF	156
RbCl	118
RbBr	88
RbI	77
CsCl <sup>(2)</sup>	99
CsBr <sup>(2)</sup>	74
CsI <sup>(2)</sup>	62

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$\nu_{\text{TO}}$  = Frequency of transverse lattice vibration

1. S. S. Mitra and P. J. Giellisse, "Infrared Spectra of Crystals," AFCRL-69-395, June (1965).
2. C. M. Randall, R. M. Fuller and D. J. Montgomery, Solid State Comm., 2, 273 (1964).

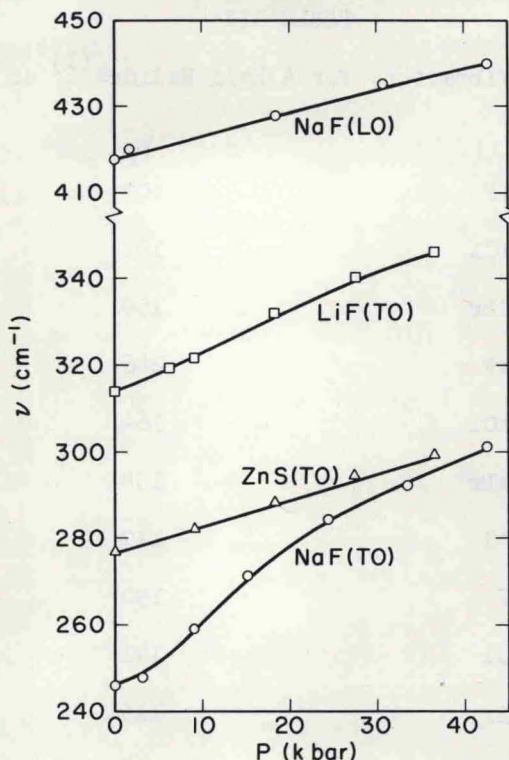


Fig. 1. Pressure Dependencies of Several Lattice Vibrations.

bility of the solid and  $\nu$  is the frequency of the particular lattice mode. For non-compressible solids it is possible that only small shifts will occur. For example, the lattice modes of zirconia and hafnia failed to show significant shifts at 40 kbars.<sup>9</sup>

The data obtained from studies of the pressure dependency of the  $k \sim 0$  lattice vibrations of ionic crystals<sup>21</sup> when combined with data from studies of these modes with temperature,<sup>22</sup> can give a better understanding of the anharmonic interactions in these solids. It is possible to distinguish between the purely volume-dependent contribution and the contribution from various anharmonic terms in the crystal Hamiltonian.<sup>23</sup> Figure 3 shows a plot of  $\ln \nu / \nu_0$  vs.  $\ln v / v_0$  for several optic modes. The data has been obtained from pressure and high temperature studies,<sup>21-23</sup> P-V data from Drickamer<sup>24</sup> and from Cline and Stephens.<sup>25</sup> It can be observed that the straight line extrapolated from the pressure domain does not coincide with the line obtained from the temperature data. The difference may be attributed to the anharmonic contribution to the frequency shift (known as the "self-energy" shift), and increases steadily with increasing temperature for