

TABLE 19

Lattice vibrations for IV—IV compounds<sup>a</sup>

	$\nu_{\text{TO}}$ ( $\text{cm}^{-1}$ )	$\nu_{\text{LO}}$ ( $\text{cm}^{-1}$ )
Diamond	1332 <sup>b</sup>	1332 <sup>b</sup>
Silicon	520 <sup>b</sup>	520 <sup>b</sup>
Germanium	301 <sup>b</sup>	301 <sup>b</sup>
SiC	793 <sup>c</sup>	970 <sup>c</sup>

<sup>a</sup> From S.S. Mitra, AFCRL-69-0468, Air Force Cambridge Research Labs., Oct. 1969.<sup>b</sup> Raman frequencies. <sup>c</sup> IR frequencies.

solid, and  $\nu$  is the frequency of the lattice mode. For non-compressible solids, it is possible that only small shifts will occur. For example, the lattice modes of zirconium and hafnium oxides failed to show significant shifts at 40 kbar [67]. It is also possible that the pressure effects may be different in noncubic crystals having different axes parameters, depending on which axis becomes compressible [172,173].

The data obtained from studies of the pressure dependence of the  $\kappa \simeq 0$

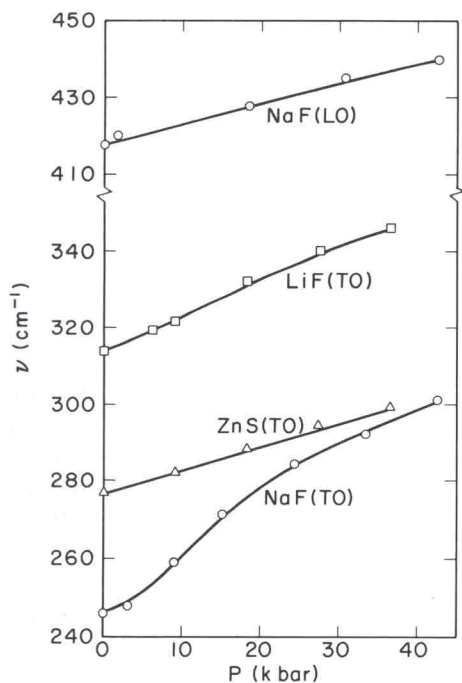


Fig. 10. Pressure dependencies of several lattice vibrations [139]. (Figure reproduced through the courtesy of the authors and Academic Press, New York.)

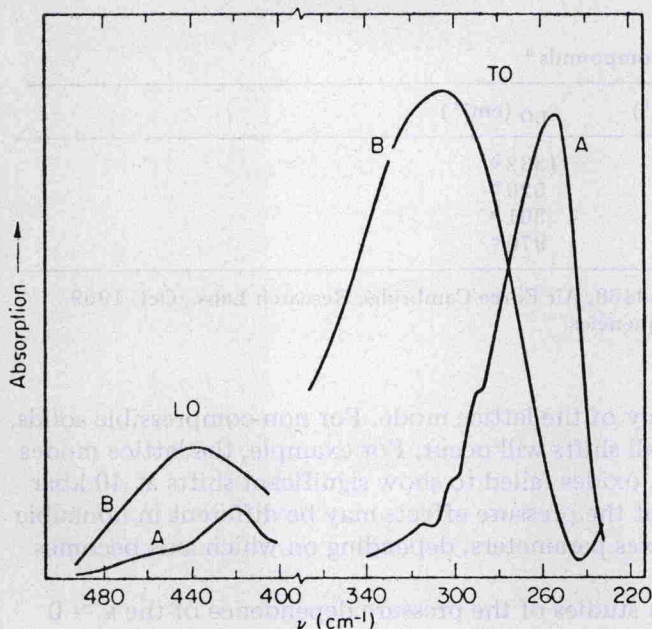


Fig. 11. Comparison of TO and LO modes in NaF with and without pressure [139]. (Figure reproduced through the courtesy of the authors and Academic Press, New York.)

lattice vibrations of ionic crystals [174], when combined with data from studies of these modes with temperature [175], may allow calculation of the anharmonic interactions taking place, and contribute to a better understanding of the lattice dynamics of these solids. It is possible to distinguish between the purely volume-dependent contribution and the contribution from various anharmonic terms in the crystal Hamiltonian [176]. Fig. 12 shows a plot of  $\ln \nu/\nu_0$  vs.  $\ln V/V_0$  for several optical modes. The data have been obtained from pressure and high-temperature studies [174–176],  $P$ - $V$  data from Pagannone and Drickamer [177], and from Cline and Stephens [178]. 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), which increases steadily with increasing temperature of LiF. A similar analysis was made for KBr and in this crystal the self-energy shift is negligible. Results obtained for RbI using other techniques [175,179] also indicated negligible self-energy shifts.

The results obtained for the Grüneisen parameters for the long-wavelength optical modes from eqns. (1) and (2)

$$\lambda_{j(k)} = -\partial \ln \nu_j(k) / \partial \ln V \quad (2)$$

are given in Table 20. The agreement with the calculations made from those