

simple cubic polonium, where Te and Se are viewed as points in a continuous distortion from the simple cubic lattice. This distortion is described in terms of the ratio between the nearest distance between atoms on different chains R to the nearest neighbour distance r within a chain [2, 5, 6]. In this picture, it becomes quite clear that with the progression towards heavier atoms (i.e., with decreasing R/r), the interchain forces increase at the expense of the intrachain forces, for ultimately to become equivalent in the case of simple cubic polonium. However, the distortion parameter R/r also decreases in Se and Te with hydrostatic pressure, allowing the pressure data obtained here and earlier to find their natural explanation within this general picture. Quantitatively, these pressure data permit investigation of the changes in the various force constants with small reductions in the distortion. As an example, we have shown elsewhere [9] that the elastic constant combination $C_{11} + C_{12}$, which describes a radial distortion in the basal plane of the trigonal crystal can, to a good approximation, be related to the single force constant K_R between nearest neighbour atoms on different chains. The assumption made is that the nearest neighbour distance within the chain r is rigid, and that we have only central forces between the chains. This expression is

$$C_{11} + C_{12} = \frac{2\sqrt{3}}{c} \left(\frac{a}{R}\right)^2 \left(1 - \frac{3}{2}x\right)^2 K_R, \quad (6)$$

where x (0.2254 for Se and 0.2633 for Te) is the internal position parameter (xa is the chain radius). Using a simple power law expression $K_R \sim R^\alpha$ we find that owing to the rapid increase in $C_{11} + C_{12}$ with pressure, the power α must be about -14 for Se and -20 for Te!

With similar assumptions, but including an intrachain bond bending force constant K_θ we arrive at the following expression for C_{33} :

$$C_{33} = \sqrt{3} \left(\frac{1}{9xa}\right)^2 \frac{c^2}{a^2} \left[K_R \left(\frac{a}{R}\right)^2 + 2K_\theta \left(\sin \frac{\theta}{2}\right)^{-2} \right], \quad (7)$$

where θ (103.06° for Se and 103.23° for Te) is the intrachain bond angle. With the above result for K_R we find the values for the logarithmic derivatives $(a/K_\theta) (dK_\theta/da)$ to be very small for Se and about four for Te.

This demonstrates how the typical interchain force constant K_R increases drastically with pressure. The intrachain bond bending force constant K_θ clearly decreases in Te with pressure in agreement with the rough estimates given in [1]. For Se a good evaluation of this quantity was difficult owing to large inconsistencies between the elastic constants, linear compressibilities, and volume compressibilities [8, 18, 20 to 22]. Clearly accurate compressibility measurements on single crystalline samples in a true hydrostatic environment are needed for such an anisotropic material as Se. The compressibilities used are given in Table 1 (footnote d). The failure to demonstrate a definite decrease in K_θ with pressure for Se can partly be ascribed to the uncertainty in the compressibilities used; but, more likely, a more sophisticated force constant model is needed to express properly the elastic constant C_{33} . However, the experiments show that the elastic constant C_{33} , which contains the highest admixture of intrachain force constants, has the smallest increase with pressure of all the elastic constants measured (see Fig. 1 and 2 and Table 1), lending further evidence to the general ideas stated earlier.

5. Study of the Homology between Se and Te

We now consider the possibility of relating the vibrational spectra in Se and Te in a fashion similar to the one used by Kucher [10], Mostoller [11], and Nilson and Nelin [12] for the group IVb elements.

As mentioned earlier, only a simple scaling of mass, force constants, and lattice parameter suffices for the higher symmetry elements of the diamond type. It was further agreed that of the two extra parameters defining the trigonal Se (Te) lattice, only the difference in c/a -ratio was of significance, and that this could be controlled by hydrostatic pressure.

We shall now consider in detail how the transformations $\text{Se} \rightarrow \text{Te}$ and $\text{Te} \rightarrow \text{Se}$ are performed. The c/a -ratios in Se and Te are 1.14 and 1.33, respectively. The pressure dependence of c/a has been measured by Vereshagin et al. [8] for Se and by Jamieson and McWhan [23] for Te. Their results show that to perform the transformation $\text{Se} \rightarrow \text{Te}$, i.e., to make $(c/a)_{\text{Se}}(p_{\text{Se}}) = (c/a)_{\text{Te}}(0)$ we arrive at the positive pressure $p_{\text{Se}} \approx 40$ kbar. Likewise, for the transformation $\text{Te} \rightarrow \text{Se}$, we find the negative pressure $p_{\text{Te}} = -35$ kbar. To obtain these values the pressure dependence of c/a and a were fitted with parabolas. This was necessary in order to account for the nonlinearity in these quantities within the pressure range of interest. To make the fits we chose three representative points from each of the experimental data sets. These are shown in Table 3. Owing to the

Table 3

Data used to make parabolic fits to the dependence of c/a and a on pressure in Se and Te. The lowest row for each element (A) shows the pressure necessary to make $(c/a)_{\text{A}}(p_{\text{A}}) = (c/a)_{\text{B}}(0)$, where B is the other element

Se			Te		
p (kbar)	c/a	a (Å)	p (kbar)	c/a	a (Å)
0	1.135	4.366	0	1.33	4.474
7.5	1.172	4.217	22.5	1.40	4.276
15.0	1.209	4.114	35.8	1.423	4.218
40	1.33	3.824	-35	1.135	5.029

small pressure range of reference [8], which seems the most reliable for Se, the values obtained for Se are somewhat uncertain (± 5 kbar for p_{Se}).

The last step in the transformation is to scale the pressurized materials by the mass ratio, and by the single lattice constant a (or c).

We now apply this transformation to the lattice vibrations, and consider first the long-wavelength optical modes. Thus, for equivalent phonons in the two lattices A and B we arrive at the following relationship:

$$\omega_{\text{A}}^2(0) = \omega_{\text{B}}^2(p_{\text{B}}) S_{\text{B} \rightarrow \text{A}} \frac{M_{\text{B}}}{M_{\text{A}}}, \quad (8)$$

where

$$\omega_{\text{B}}^2(p_{\text{B}}) = \omega^2(0) + k_1^{\text{B}} p_{\text{B}} + k_2^{\text{B}} p_{\text{B}}^2 + \dots \quad (9)$$