

Here p_B represents the pressure needed to fulfil the condition $(c/a)_B(p_B) = (c/a)_A(0)$ and is given above for Te and Se. M_B and M_A are the respective masses for the atoms A and B. $S_{B \rightarrow A}$ is the ratio of the equivalent zero-pressure force constant $K_A(0)$ in the material A and that of material B $K_B(p_B)$ under pressure p_B , i.e. $S_{B \rightarrow A} = K_A(0)/K_B(p_B)$. We note that the scaling of the unit cell does not enter into (8) for the optical modes due to their lack of dispersion at long wavelengths. The experimental Raman frequencies and their pressure coefficients are listed in Table 4. The long-wavelength acoustical modes are most conveniently discussed in terms of the ultrasonic velocities. As a conse-

Table 4

Raman modes: $\omega(0)$ frequencies under atmospheric pressure; k_1 first-order pressure coefficient of ω^2 (equation (9)); S_i mode force constant ratios obtained from the transformations Se \rightarrow Te and Te \rightarrow Se using first-order expansion in pressure (S_1) and second-order expansion (S_2). $k_2^{\text{Te}} = k_2^{\text{Se}} = k_2$ is the approximation used in the second-order expansion (see equation (9))
 $S_1 = K_{\text{Te}}(0)/K_{\text{Se}}(40)$ or $K_{\text{Te}}(-35)/K_{\text{Se}}(0)$

mode	$\omega(0)$ (cm ⁻¹)		k_1 (cm ⁻² /kbar)		$S_1 = S_{\text{Se} \rightarrow \text{Te}}$	$S_1 = S_{\text{Te} \rightarrow \text{Se}}^{-1}$	$S_2 = S_{\text{Se} \rightarrow \text{Te}}$ $= S_{\text{Te} \rightarrow \text{Se}}^{-1}$	$k_2 = k_2^{\text{Te}} = k_2^{\text{Se}}$ (cm ⁻² /kbar ²)
	Te *)	Se *)	Te *)	Se *)				
A ₁	121.0	238.6	-218	-305	0.53	0.63	0.57	-1.9
E''	141.4	235.8	-139	-90	0.62	0.72	0.66	-1.8
E'	92.8	148.6	-13	-21	0.66	0.66	0.66	-0.1

*) Values obtained from [1].

quence of the linear dispersion in these we obtain for the transformation B \rightarrow A

$$v_A^2(0) = v_B^2(p_B) S_{B \rightarrow A} \frac{M_B}{M_A} \left(\frac{l_A(0)}{l_B(p_B)} \right)^2, \quad (10)$$

where

$$v_B^2(p_B) = v_B^2(0) + k_1^B p_B + k_2^B p_B^2 + \dots; \quad (11)$$

$l(p)$ represents either of the lattice parameters a or c at the pressure shown in the parenthesis. The presence of $l(p)$ reflects the linear dispersion in the acoustical modes in the ultrasonic region. The experimental sound velocities v_0 and the pressure coefficients k_1 are listed in Table 5.

As mentioned, the transformation equations (8), (9) and (10), (11) can be carried out either as Se \rightarrow Te or Te \rightarrow Se. However, to claim a homological relationship between the vibrational modes in Se and Te for each of these transformations we must require that the force constant ratio $S_{B \rightarrow A}$ must be the same for all modes in the two species. Here we only consider zone centre modes; however, these involve a number of inter- and intrachain force constants, and should therefore serve as a good testing ground for the idea. We further expect some degree of reciprocity in the two transformations Se \rightarrow Te and Te \rightarrow Se in the sense that $S_{B \rightarrow A} = S_{A \rightarrow B}^{-1}$. For a simple representation of force constants by one-term power laws in the lattice parameter a and c , it can be shown (Appendix A) that this indeed seems to be the case. This point will, however, be further studied in the course of the discussion of the experimental data on the individual modes.

Table 5

Ultrasonic waves: v_0 sound velocities under atmospheric pressure; k_1 first-order pressure coefficients of v^2 (equation (11)); S_i ultrasonic force constant ratios obtained from the transformations Se \rightarrow Te and Te \rightarrow Se. The first-order pressure expansion (S_1) is only applicable for Se \rightarrow Te, and for the $\mathbf{q} \parallel Z$ -direction for Te \rightarrow Se (see text). Again, the approximation $k_2^{\text{Se}} = k_2^{\text{Te}} = k_2$ is used in the second-order expansion (S_2)

mode *)	v_0 (10^5 cm/s)		k_1 (10^{10} cm ² /s ² kbar)		$S_1 =$	$S_1 =$	$S_2 =$	$k_2 =$
	Te	Se	Te	Se	$S_{\text{Se} \rightarrow \text{Te}}$	$S_{\text{Te} \rightarrow \text{Se}}^{-1}$	$S_{\text{Se} \rightarrow \text{Te}} = S_{\text{Te} \rightarrow \text{Se}}^{-1}$	$= k_2^{\text{Te}} = k_2^{\text{Se}}$ (10^6 cm ² /s ² kbar ²)
L(Z)	3.36	4.14	0.143	0.194	0.54	0.44	0.52	8.7
T(Z)	2.26	1.95	0.100	0.157	0.61	0.51	0.61	2.0
L(X)	2.30	2.00 **)	0.172	0.169 **)	0.59		0.46	18.5
FT(X)	2.42	2.10 **)	0.132	0.182 **)	0.61		0.55	6.5
ST(X)	0.98	1.05 **)	0.021	0.030 **)	0.50		0.46	1.6
QL(Y)	2.66	2.28	0.197	0.221	0.61		0.51	16.5
QT(Y)	1.79	1.61	0.080	0.105	0.57		0.50	5.5
T(Y)	1.42	1.31	0.056	0.056	0.61		0.50	5.4

*) The symbols in this column are explained in Table 1.

***) These values are calculated from the results for the Z- and Y-directions.

It is clear from the magnitude of the pressures needed for the transformations that one cannot, in general, expect a simple linear behaviour in the squared lattice frequencies over such pressure ranges. This can be seen from the experimental information on the lattice parameters (and the c/a -ratio) versus pressure. As will be evident this poses certain problems, particularly in the discussion of the acoustical modes. However, with due consideration to this difficulty, we shall now proceed to evaluate our data within the framework of the ideas presented here.

6. Discussion

6.1 Discussion of the optical modes

The force constant ratio $S = S_{B \rightarrow A}$ of (8) is obtained from pressure expansion of $\omega^2(p)$ as shown in (9). Only the first-order expansion coefficient k_1 is known experimentally; and with this linear approximation we obtain the values for S_1 shown in Table 4 for the two independent transformations Se \rightarrow Te and Te \rightarrow Se. We have used the notation $S_1 = S_{\text{Se} \rightarrow \text{Te}}$ and $S_1 = S_{\text{Te} \rightarrow \text{Se}}^{-1}$ for the two transformations, respectively. We note that the agreement between the two values is in each case quite good. This shows (i) that for the optical modes the linear approximation is quite reasonable for ω^2 versus pressure, and (ii) that the reciprocity condition $S_{B \rightarrow A} = S_{A \rightarrow B}^{-1}$ is a quite reasonable one. The order of magnitude of the nonlinearity (i.e., k_2) in the pressure dependence of ω^2 can be estimated by making the rough approximation that $k_2^{\text{Te}} = k_2^{\text{Se}} = k_2$. Then, the two transformation relationships can be solved simultaneously for k_2 and S (now labelled $S_2 = S_{B \rightarrow A} = S_{A \rightarrow B}^{-1}$), giving the values shown also in Table 4. We note that S_2 is intermediate between the two independent estimates of S_1 . Further, we see that the coefficients k_2 are indeed small; predicting a very slight deviation from linearity in ω^2 over all pressure ranges of interest here. The sign