Table 1

Effective elastic constants and their logarithmic pressure derivatives for Se and Te

mode[a])	C (10^{11} dyn/cm^2)					$\frac{1}{C}\frac{dC}{dp}$[d]) (10^{-2} kbar^{-1})	
	Te		Se			Te	Se
	this work	ref. [17]	this work	ref. [19]	ref. [18]		
L(Z), C_{33}	7.05	7.22	8.20	8.02	7.41	1.79	2.1
T(Z), C_{44}	3.19	3.12	1.82	1.83	1.49	2.47	5.1
L(X), C_{11}	3.30	3.27	1.91[b])		1.87	3.78	5.2[e])
FT(X), C_2	3.66	3.72	2.12[b])		1.80	2.77	5.1[e])
ST(X), C_3	0.60	0.60	0.52[b])		0.24	2.74	3.7[e])
QL(Y), C_4	4.40	4.42	2.49		2.33	3.30	5.2
QT(Y), C_5	2.00	1.95	1.24		1.03	3.01	5.0
T(Y), C_{66}	1.25	1.21	0.82		0.55	3.30	4.2
$\lvert C_{14}\rvert$	1.19[b])	1.24	0.62[b])		0.62		
C_{13}	2.31[c])	2.49	2.3[c])		2.60		

[a]) Designations: L longitudinal, T transverse, FT fast transverse, ST slow transverse, QL quasi-longitudinal, QT quasi-transverse, (X), (Y), (Z) direction of phase velocity; C_2 to C_5 are defined in equations (1) and (2).

[b]) Calculated from equations (1) and (2).

[c]) Calculated from the volume compressibilities: Te: 0.52×10^{-11} cm^2/dyn [7]; Se: 0.94×10^{-11} cm^2/dyn [9].

[d]) The linear compressibilities used are (in units of 10^{-3} kbar^{-1}): $-\frac{1}{a}\frac{da}{dp} = 2.8$ (Te), 5.7 (Se); $-\frac{1}{c}\frac{dc}{dp} = -0.4$ (Te), -2.0 (Se) [7 to 9]. Due to the relative large uncertainty in the compressibilities of Se the pressure derivatives in this column can have an uncertainty of as much as 25% for C_{33}; but typically less than 10% for the basal plane modes.

[e]) Calculated from equations (3) to (5).

for the quasi-longitudinal (+) and quasi-transverse (−) modes in the Y-direction. (Note that the relationship given in reference [17] for C_2C_3 is obviously in error.) With the present elastic constants and the volume compressibility by Bridgeman [7] (0.52×10^{-11} cm^2/dyn), we obtain a value for C_{13} as shown in Table 1.

For Se there exists in the literature a complete set of elastic constants by Mort [18], and measurement only along the trigonal axis (i.e., C_{33} and C_{44}) by Vedam et al. [19]. Our data for the latter are in very good agreement with those by Vedam et al. but Mort's values are lower by 10 to 20%. This is typical for his data when compared with the present ones, also for the X- and Y-direction. Our agreement with Vedam et al. for the Z-direction in Se, and the good agreement with Malgrange et al. for Te together with the fact that we performed all our measurements consistently, without variation in technique, lead us to believe that our data for the elastic constants in Se along with those of Vedam et al. are the more accurate. Using the present data, and a volume compressibility of 0.94×10^{-11} cm^2/dyn (see [7] and the discussion in Section 4) we obtain an estimate for C_{13} (see Table 1) in Se.

Table 2

Consistency checks on the elastic constants and on their pressure derivatives in Te (see equations (3) to (5) in the main text). The elastic constants have the units (10^{11} dyn/cm^2)

$C_2 + C_3$	$= 4.26$	$K_2 + K_3$	$= 11.8$
$C_{44} + C_{66}$	$= 4.44$	$K_{44} + K_{66}$	$= 12.0$
$C_4 + C_5$	$= 6.40$	$K_4 + K_5$	$= 20.5$
$C_{11} + C_{44}$	$= 6.49$	$K_{11} + K_{44}$	$= 20.4$
$[(C_2 - C_3)^2 - (C_4 - C_5)^2]^{1/2}$	$= 1.90$	$[(C_2 - C_3)(K_2 - K_3) - (C_4 - C_5)(K_4 - K_5)]^{1/2}$	$= 2.4$
$[(C_{44} - C_{66})^2 - (C_{44} - C_{11})^2]^{1/2}$	$= 1.91$	$[(C_{44} - C_{66})(K_{44} - K_{66}) - (C_{44} - C_{11})(K_{44} - K_{11})]^{1/2}$	$= 2.6$

The three redundancies in measurement of the absolute values and of the pressure coefficients for the elastic constants in Te allow us to perform three checks on internal consistency for both. Using the notation C_α and $K_\alpha = (\mathrm{d}/\mathrm{d}p)C_\alpha$ for the absolute values and the pressure coefficients of the elastic constants respectively, we have the following relationships:

$$C_{44} + C_{66} = C_2 + C_3\,, \qquad K_{44} + K_{66} = K_2 + K_3\,, \tag{3}$$

$$C_{44} + C_{11} = C_4 + C_5\,, \qquad K_{44} + K_{11} = K_4 + K_5\,, \tag{4}$$

$$\left.\begin{aligned} [(C_{44} - C_{66})^2 - (C_{44} - C_{11})^2]^{1/2} &= [(C_2 - C_3)^2 - (C_4 - C_5)^2]^{1/2} \\ [(C_{44} - C_{66})(K_{44} - K_{66}) - (C_{44} - C_{11})(K_{44} - K_{11})]^{1/2} &= \\ = [(C_2 - C_3)(K_2 - K_3) - (C_4 - C_5)(K_4 - K_5)]^{1/2}\,. & \end{aligned}\right\} \tag{5}$$

The two-digit subscripts reflect the conventional notation, while C_α ($\alpha = 2, \ldots, 5$) are defined in (1) and (2). The square root signs in (5) are retained to preserve consistency with (3) and (4) in evaluating the errors.

Table 2 shows that the internal consistency in our measurements is quite satisfactory, with a maximum error of 4% in the elastic constants and in their pressure derivatives. This is also in agreement with the maximum uncertainty expected in our experiments. The larger relative discrepancy in the lower of (5) is merely due to the near cancellation of large numbers inside the square brackets. A similar uncertainty is also expected for the experimental data on Se. However, the lack of reliable values for the linear compressibilities introduces relatively large uncertainties in some of the logarithmic pressure derivatives of the elastic constants (see footnote in Table 1).

4. Atomic Force Constants and the Pressure Dependence of the Lattice Vibrations

As mentioned earlier, the qualitative features of the pressure dependence of the long-wavelength optical and acoustical vibrations finds a natural explanation in the ideas put forward, in particular by Martin and Lucovsky [5, 6]. The optical modes tend to soften and acoustical modes stiffen due to the weakening of the strong intrachain covalent bonds owing to transfer of electronic charge to the weak interchain bonds as the chains are packed closer together. This can be seen in the larger context of a progression from molecular sulfur to metallic