TABLE I. Adiabatic elastic constants of $RbAg_4I_5$ at 25 °C and their temperature and pressure derivatives based on the measured natural wave velocities. The first three entries in each column were directly determined experimentally, and the other entries were calculated from them.

	C_{ij} (10^{11} dyn/cm^2)	$\frac{1}{\rho_0 W^2}\frac{\partial(\rho_0 W^2)}{\partial T}$ (10^{-4} °K^{-1})	$\frac{\partial(\rho_0 W^2)}{\partial P}$
C_L	1.780 ± 0.002	−3.19 ± 0.10	+7.85 ± 0.08
C'	0.3568 ± 0.0003	−2.72 ± 0.02	+1.115 ± 0.010
C_{44}	0.4892 ± 0.0005	−3.60 ± 0.05	+0.734 ± 0.015
C_{11}	1.648 ± 0.002	−2.97 ± 0.12	+8.23 ± 0.11
C_{12}	0.934 ± 0.002	−3.16 ± 0.13	+6.00 ± 0.11
K	1.172 ± 0.003	−3.07 ± 0.13	+6.74 ± 0.11

$$\frac{1}{C}\left(\frac{\partial C}{\partial T}\right)_P = \frac{1}{\rho_0 W^2}\left(\frac{\partial(\rho_0 W^2)}{\partial T}\right)_P - \alpha, \tag{1}$$

$$\left(\frac{\partial C}{\partial P}\right)_{T,P=0} = \left(\frac{\partial(\rho_0 W^2)}{\partial P}\right)_{T,P=0} + \frac{C}{3K^T}, \tag{2}$$

where C is the adiabatic elastic modulus in question, α is the linear thermal expansion coefficient, and K^T is the isothermal bulk modulus. This can be obtained from the relation[9]

$$\frac{K^S}{K^T} = 1 + \frac{9\alpha^2 K^S T}{\rho C_p}. \tag{3}$$

An approximate value of $\alpha = 0.57\times10^{-4}$ °K^{-1} was obtained from lattice parameter measurements at 25 °C and −50 °C.[10] Using a value of the heat capacity $C_p = 0.0593$ cal/g °K,[7] $K^S/K^T = 1.077$, and $K^T = 1.089\times10^{11}$ dyn/cm^2. These values of α and K^T can be used in Eqs. (1) and (2) to convert the values of the temperature and pressure derivatives shown in Table I to the true values with very little error. These are shown in Table II.

There are several bulk property values that can be calculated from the single-crystal elastic constants. The elastic properties of an isotropic polycrystalline solid of the same material are often required since technological use of the polycrystalline material is more common than of the single crystal. An approximation to the polycrystalline values can be obtained from the single-crystal elastic constants using the Voigt-Reuss-Hill[11] or the Hashin-Shtrikman[12] methods. For $RbAg_4I_5$ both methods yield the same values for Young's modulus, shear modulus, and Poisson's ratio which are $E = 1.155\times10^{11}$ dyn/cm^2, $G = 0.432\times10^{11}$ dyn/cm^2, and $\nu = 0.336$ at 25 °C.

Using these values for the average bulk elastic properties, the Debye characteristic temperature can be calculated.[13] This was in fact done at three temperatures, 25, −68, and −110 °C which resulted in the values for θ_D of 90.8, 90.3, and 92.5 °K, respectively. These values should be within a few percent of the value determined calorimetrically if the elastic behavior of the low-temperature phase is not too different from that of the high-temperature phases. The specific-heat data result in a Debye temperature of 92 °K,[7] which suggests that this is indeed the case.

Another bulk property value which can be calculated from the single-crystal elastic constants and their pressure derivatives is the Grüneisen parameter, γ. The thermal expansion coefficient at 25 °C can be obtained from this value through the relation

$$\alpha = \rho C_p \gamma / 3K^S \tag{4}$$

for comparison with the approximate value used in the previous calculations. An estimate of its temperature dependence could also be obtained from the temperature dependence of C_p,[7] since the other parameters in this relation are relatively insensitive to temperature. This could be used with the data of Figs. 1–3 to obtain a better estimate of the temperature dependence of the single-crystal elastic constants, if this was desired.

In the Debye model, a Grüneisen parameter can be expressed in terms of the second- and third-order elastic constants for each of the standing wave modes of the elastic continuum. The Grüneisen parameter which describes the average bulk properties can be obtained by the appropriate averaging over all possible wave modes. In lieu of this for a crystal with cubic symmetry, an approximation can be made by averaging over only the 39 pure-wave modes which can propagate in the directions of the cube edges and the face and body diagonals. The expressions for the mode γ's associated with each of these waves have been derived previously.[14] Instead of taking the sum of all of these mode γ's, we sum the ones associated with longitudinal and shear modes separately resulting in the equations

$$\gamma_L = -\frac{1}{13}\left(\frac{3C_{11}+2C_{12}+C_1}{2C_{11}} + \frac{2(5C_{11}+10C_{12}+8C_{44}+3C_1+4C_2-4C_3)}{3(C_{11}+2C_{12}+4C_{44})} + \frac{2(2C_{11}+3C_{12}+2C_{44}+C_1+C_2-C_3)}{C_{11}+C_{12}+2C_{44}}\right), \tag{5}$$

$$\gamma_S = -\frac{1}{26}\left(\frac{2(C_{11}+2C_{12}+2C_{44}+C_2)}{C_{44}} + \frac{4(5C_{11}+4C_{12}+2C_{44}+C_2+2C_3)}{3(C_{11}-C_{12}+C_{44})} + \frac{2(2C_{11}+C_{12}+C_3)}{C_{11}-C_{12}}\right), \tag{6}$$

TABLE II. Temperature and pressure derivatives of the adiabatic second-order elastic constants of $RbAg_4I_5$ at 25 °C and 1 atm pressure.

	$\frac{1}{C}\left(\frac{\partial C}{\partial T}\right)_P$ (10^{-4} °K^{-1})	$\left(\frac{\partial C}{\partial P}\right)_{T,P=0}$
C_{11}	−3.54 ± 0.12	+8.73 ± 0.11
C_{12}	−3.73 ± 0.13	+6.29 ± 0.11
C_{44}	−4.17 ± 0.05	+0.884 ± 0.015
C_L	−3.76 ± 0.10	+8.40 ± 0.08
C'	−3.29 ± 0.02	+1.224 ± 0.010
K	−3.64 ± 0.13	+7.10 ± 0.11

where the C_{ij} are the adiabatic second-order elastic constants, and the C_i are the combinations of third-order elastic constants $C_1 = C_{111} + 2C_{112}$, $C_2 = C_{144} + 2C_{166}$, and $C_3 = \frac{1}{2}(C_{111} - C_{123})$. These combinations of the third-order elastic constants are determined uniquely by the hydrostatic pressure derivatives of the second-order constants shown in Table I.[8] Their values in the units of 10^{12} dyn/cm^2 are $C_1 = -3.30$, $C_2 = -0.656$, and $C_3 = -0.752$. For temperatures greater than θ_D,

$$\gamma = \tfrac{1}{3}(\gamma_L + 2\gamma_S). \tag{7}$$

Evaluating Eqs. (5)–(7) results in $\gamma = 1.49$, and using this value in Eq. (4) gives $\alpha = 0.566 \times 10^{-4}\,^{\circ}\mathrm{K}^{-1}$ which agrees with the value $0.57 \times 10^{-4}\,^{\circ}\mathrm{K}^{-1}$ determined from lattice parameter measurements. This agreement validates the calculated temperature and pressure derivatives of the elastic constants shown in Table II.

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