But,

$$q \propto (L_1^2 + L_2^2 + L_3^2)^{-1/2} \quad (6)$$

where L_1, L_2 and L_3 are the lengths of the crystal parallel to the x, y and z axes, and $s_p(\theta, \phi)$ is the sound velocity for the mode $\mathbf{q}, p$. Hence, one obtains the relation:

$$[\partial \ln \omega_p(\mathbf{q})/\partial P]_T = (l^2 K_1^T + m^2 K_2^T + n^2 K_3^T) + [\partial \ln s_p(\theta, \phi)/\partial P]_T \quad (7)$$

where K_1^T, K_2^T and K_3^T are the isothermal linear compressibilities in the directions of the crystalline axes, and l, m, n, are the *direction cosines of* $\mathbf{q}$. Denoting the elastic stiffness modulus associated with the mode q, p by c_p, one obtains:

$$(\partial \ln \omega_p(\mathbf{q})/\partial P) = l^2 K_1^T + m^2 K_2^T + n^2 K_3^T - 0{\cdot}5\, K_V^T + 0{\cdot}5(\partial \ln c_p/\partial P)_T \quad (8)$$

where K_V^T is the isothermal volume compressibility. Thus, we have

$$\sum_{i,j=1}^{3} s_{ij}\gamma_j^p(\mathbf{q}) = l^2 K_1^T + m^2 K_2^T + n^2 K_3^T - 0{\cdot}5 K_V^T + 0{\cdot}5(\partial \ln c_p/\partial P)_T. \quad (9)$$

Defining now an averaged mode gamma

$$\gamma^p(\mathbf{q}) = \left(\sum_{i,j=1}^{3} s_{ij}\right)^{-1} \times \left[\sum_{i,j=1}^{3} s_{ij}\gamma_j^p(\mathbf{q})\right] \quad (10)$$

one obtains

$$\gamma^p(\mathbf{q}) = [l^2 K_1^T + m^2 K_2^T + n^2 K_3^T - 0{\cdot}5 K_V^T + 0{\cdot}5(\partial \ln c_p/\partial P)_T] \Big/ \left(\sum_{i,j=1}^{3} s_{ij}\right). \quad (11)$$

As can be seen the individual mode gammas $\gamma_i^p(\mathbf{q})$ cannot be deduced from the pressure derivatives of the elastic moduli alone, but only their weighted average. In order to determine the individual $\gamma_i^p(\mathbf{q})$, uniaxial as well as hysrostatic pressure derivatives of the elastic moduli are required.

The Grüneisen parameter, defined by

$$\gamma = \beta V \Big/ \left(C_V \sum_{i,j=1}^{3} s_{ij}\right) \quad (12)$$

where β is the volume expansion thermal expansion coefficient ($\beta = \alpha_1 + \alpha_2 + \alpha_3$), C_V the specific heat at constant volume V, is given by[7]

$$\gamma = \left[\sum_{q,p} C_p(\mathbf{q})\gamma^p(\mathbf{q})\right] \Big/ \left[\sum_{q,p} C_p(\mathbf{q})\right] \quad (13)$$

where $C_p(\mathbf{q})$ is the specific heat associated with the mode $\mathbf{q}.p$. The low and high temperature limits of the Grüneisen parameter, γ_L and γ_H may be easily calculated, as at the low temperature limit $C_p(\mathbf{q}) \propto c_p^{-3/2}$, while in the high temperature limit $C_p(\mathbf{q}) = kT$. Hence, in these two limiting cases the sum in equation (13) may be evaluated in a straight forward manner.

A computer program for the CDC 3600 computer which evaluates the averaged mode gammas $\gamma^p(\mathbf{q})$, as well as γ_L and γ_H in crystals of cubic, hexagonal, tetragonal and orthorhombic symmetry has been written. The input data to the program are the room temperature elastic moduli, their pressure derivatives, and the low temperature elastic moduli. The program computes the sound velocity in any direction by calculating the eigenvalues of the Christoffel determinant[8], as well as the pressure derivatives in any direction. From the latter quantities the $\gamma^p(\mathbf{q})$ as function of direction are determined. γ_L and γ_H are evaluated by numerical quadrature.*

The above program has been applied to three materials of hexagonal symmetry, where the values of the elastic moduli and their pressure derivatives are available, i.e. magnesium[9, 10], cadmium[11, 12] and cadmium sulfide[13, 14]. Since the hexagonal structure has transverse symmetry, the $\gamma^p(q)$ need only be evaluated as a function of the latitude angle θ. The results of the computation are shown in Figs. 1–3, where $p = 1$ is the longitudinal mode, $p = 2$ the fast shear mode, and

*A write-up of the program may be obtained from the author upon request.