Mg_2Si and Mg_2Ge.) Such a small charge is consistent with the covalent nature of the bonding in these compounds, yet it is large enough to account for the infrared reflectivity spectrum which is characteristic of an ionic compound.

Calculations of the lattice vibration frequencies in Mg_2Sn could be compared with experiment only by comparing the calculated and experimental Debye curves. Good agreement was attained when the polarizability of the Sn was taken into account. The sharp minimum in the Debye temperature near 20°K was found to be due to a low-lying transverse acoustic mode. Inelastic neutron scattering has revealed such a mode in Ge[18,27] and GaAs.[18,28] More experimental information, such as the Raman spectrum, multiple phonon absorption frequencies, and inelastic neutron scattering, is necessary to provide a more accurate description of the phonons in Mg_2Sn, but, the results of the present investigation are thought to give a reasonable first approximation.

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APPENDIX

Following GANESAN and SRINIVASAN[24] we define the matrix of force constants between one ion and another. The matrix can be written most generally as

$$D = \begin{pmatrix} \phi_{xx} & \phi_{xy} & \phi_{xz} \\ \phi_{yx} & \phi_{yy} & \phi_{yz} \\ \phi_{zx} & \phi_{zy} & \phi_{zz} \end{pmatrix}$$

where, for example, $\phi_{xy} = (\partial^2\phi/\partial x\partial y)$ is evaluated at the equilibrium separation. ϕ is the two-body potential associated with the short range forces between one ion and another.

We list the matrix of force constants for the Sn core–Sn shell, nearest neighbor Mg–Sn, next nearest