

Table 2
Pressure derivatives of the adiabatic elastic constants of lead at 296 and 195 °K as obtained by Miller and Schuele (M & S) and by the iterative procedure (IP)

	296 °K		195 °K	
	M&S	IP	M&S	IP
C_{11}	5.94	6.02	5.82	5.90
C_{12}	5.33	5.40	5.26	5.34
C_{44}	2.06	2.10	1.97	2.01
B_S	5.53	5.61	5.45	5.50

a solid are estimated in the above manner at the pressure P as a function of temperature, we obtain new estimates of $[\partial\chi^T(l, m, n, P, T)/\partial T]_P$ and $[\partial\beta(l, m, n, P, T)/\partial T]_P$. If these new values of $[\partial\chi^T(l, m, n, P, T)/\partial T]_P$ and $[\partial\beta(l, m, n, P, T)/\partial T]_P$ in the three principal directions agree with their respective assigned values at the beginning of the calculation the estimated values of the elastic constants at the pressure P and all the temperatures are considered correct. If these new values of $[\partial\chi^T(l, m, n, P, T)/\partial T]_P$ and/or $[\partial\beta(l, m, n, P, T)/\partial T]_P$ do not agree with their previously assigned values the iterative procedure is repeated all over again with these new values as the starting point, until two consecutive estimates of $[\partial\chi^T(l, m, n, P, T)/\partial T]_P$ and $[\partial\beta(l, m, n, P, T)/\partial T]_P$ agree with their respective values in all the three principal directions. (See the flow chart in Table 1).

The net outcome includes

- (i) the values of the elastic constants as a function of pressure and temperature,
- (ii) the values of the partial temperature and pressure derivatives of the linear thermal expansion coefficient as a function of pressure and temperature, and
- (iii) the pressure derivative of the specific heat as a function of temperature.

If, however, the transit time of the elastic waves in a solid is measured as a function of pressure at only two temperatures, then the values of the elastic constants of the solid may be estimated at high pressure by interpreting P_1 in relation (14) to signify some lower pressure at which these quantities are known, and by omitting the iterations on $[\partial\beta(l, m, n, P, T)/\partial T]_P$ in the above scheme. Lastly, if transit times of the elastic waves in a solid are measured as a function of pressure at only one temperature, then the values of the elastic constants may be estimated at high pressures by interpreting P_1 in both relations (13) and (14) to signify some lower pressures at which these quantities are known, and by omitting the iteration on $[\partial\chi^T(l, m, n, P, T)/\partial T]_P$ and $[\partial\beta(l, m, n, P, T)/\partial T]_P$ in the above scheme.

We have applied the iterative procedure described above to estimate the values of the elastic constants from the ultrasonic data for lead (a cubic solid) at 296 and 195 °K to 3 kbar [6], for rutile (a tetragonal solid) at 298 °K to 7.5 kbar [7], and for calcite (a trigonal solid) at 298 °K to 6 kbar [8]. Table 2 compares the values of the pressure derivatives of adiabatic elastic constants of lead at 296 and 195 °K as calculated by Miller and Schuele and by the itera-

Table 3

Adiabatic elastic constants (in units of 10^{11} dyn/cm²) of calcite with pressure at 298 °K as obtained by Dandekar (D) [8] and as obtained by the iterative procedure (IP) from the same ultrasonic data

Pressure (kbar)	C_{11}		C_{33}		C_{44}		C_{66}		C_{14}		C_{13}	
	D	IP	D	IP	D	IP	D	IP	D	IP	D	IP
0.001	± 0.05	14.626	± 0.05	8.531	± 0.02	3.405	± 0.07	4.328	± 0.06	± 0.33	± 0.33	5.076
2.0	14.650	14.651	8.526	8.527	3.453	3.453	4.335	4.336	-2.076	5.076	5.190	5.179
4.0	14.674	14.676	8.522	8.522	3.468	3.468	4.342	4.343	-2.078	5.190	5.419	5.402
6.0	14.697	14.700	8.518	8.516	3.449	3.448	4.349	4.350	-2.101	5.419	5.757	5.734

Sources of the values of thermodynamic parameters used in the I.P.: Thermal expansion coefficients from [10], temperature derivative of the compressibilities at one atmosphere from [11], specific heat value from [12].

Table 4

Adiabatic elastic constants (in kbar) of single crystal rutile with pressure at 298 °K obtained by Manghanani (M) [7] and by the iterative procedure (IP) from Manghanani's data

Pressure (kbar)	C_{11}		C_{33}		C_{44}		C_{66}		C_{12}		C_{13}	
	M	IP	M	IP	M	IP	M	IP	M	IP	M	IP
0.001	2714.3	2714.3	4839.5	4839.5	1244.3	1244.3	1947.7	1947.7	1779.6	1779.6	1495.7	1495.7
1.25	2722.4	2722.4	4849.9	4850.8	1245.7	1245.2	1955.7	1955.7	1791.0	1791.0	1502.0	1503.4
2.50	2730.5	2730.4	4860.3	4862.1	1247.1	1246.3	1963.8	1963.7	1802.3	1802.3	1508.3	1509.6
5.00	2746.7	2746.6	4881.2	4884.7	1249.8	1248.4	1979.9	1979.7	1825.1	1825.1	1520.8	1522.2
7.50	2762.8	2762.8	4902.0	4907.3	1252.6	1250.5	1996.0	1995.9	1847.8	1847.8	1533.4	1534.8

Sources of the values of thermodynamic parameters: Same as those used by Manghanani [7], i.e. thermal expansion coefficients from [13], specific heat value from [14], and temperature derivatives of the compressibilities at 1 atm [7].