

Table I

Parameter	195°K	0°K
B_O^T	69.26 kb	77 kb
$B_O^{T'}$	3.904	3.904*
$B_O^{T''}$	-0.0696 kb ⁻¹	-0.0696 kb ⁻¹ *

*We assume that the isothermal pressure derivatives do not vary with temperature. This is discussed by Swenson¹² for $B_O^{T'}$.

III THEORETICAL CALCULATION

In order to calculate the values of the bulk modulus and its pressure derivatives at zero pressure, we have to know the total energy of the solid as a function of volume analytically. The method proposed by Ashcroft and Langreth² is used in the present calculation. The total energy of the solid per electron (assuming a static lattice) at 0°K is expressed as:

$$E = \frac{2.21}{r_s^2} - \frac{0.916}{r_s} - (0.115 - 0.031 \ln r_s) - \frac{1.792Z}{r_s^{2/3}} + \frac{3\alpha}{4\pi r_s^3} + E_B \quad (4)$$

where $\frac{4}{3} \pi r_s^3 = v = \frac{1}{n}$ is the average volume per electron, Z is the number of free electrons per ion, $\alpha = 4\pi r_c^2$ is the parameter to be determined by the zero pressure condition $\frac{dE}{dr_s} = 0$, E_B is the contribution due to band structure effects.

Barrett¹³ first reported a partial phase transformation of sodium from bcc to hcp near 35°K. Microscopic experiments have shown such a transformation is of the martensitic type. In the present calculation, we have assumed that sodium is in the bcc