obtain the total correlation correction.)

The pressure p on the solid at a given volume V per primitive unit cell can be calculated from the non-equilibrium virial theorem [14,15],

$$p V = (< U > + 2 < T >) / 3 \quad , \qquad (1)$$

which is satisfied identically in the $X\alpha$ approximation, for the statistical ($X\alpha$) effective total potential energy $< U >$ and kinetic energy $< T >$ per primitive unit cell. Such a calculation has been performed, and the computed pressure is shown as a function of volume in Fig. 1b. As a check on the numerical accuracy of the calculation, the pressure has also been obtained from the relation

$$p = - d E / d V \qquad (2)$$

(where E is the total or cohesive energy per primitive unit cell), which is found to give results in good agreement with those shown. The bcc p-V curve is found by Averill [16] to be in good agreement with the compression measured by Swenson [17] at low temperatures.

It is in the pressure curve for fcc cesium that the first clear indication of the isomorphic phase transition appears: the curve dips, showing a clear minimum at a volume of about 350 cubic

atomic units (c.a.u.) per atom. From the fcc cohesive energy and pressure curves, the enthalpy is obtained, as illustrated in Fig. 2. (The relevant computed points are numbered in Fig. 1a, 1b, and 2, to facilitate comparison. All points with a given number correspond to a single lattice volume and pressure.) In this curve, the transition appears as the intersection of the line from point 1 to point 2, with that from 4 to 5. As the metal is compressed at 0 K, it must move along the curves from point 1 to the point of this intersection on the enthalpy curve (about 26 kbar, which corresponds to $V \approx 410$ c.a.u.), at which point it jumps to the corresponding point on the curves from point 4 to point 5 (26 kbar, and about 320 c.a.u.), following the curves to point 5. The 0 K computed isomorphic phase transition thus consists of a discontinuous volume change from approximately 410 c.a.u. to 320 c.a.u., at a pressure of roughly 26 kbar. There is no experimental data with which to compare these results at 0 K, but the volumes are in good agreement with the observed room temperature decrease from 362 c.a.u. to 329 c.a.u. [8]. The calculated pressure of 26 kbar (for 0 K) is not in such close agreement with the 42 kbar pressure observed for the transition at the higher temperatures, but the calculated pressure is subject to all the errors of the model (and is not a variational quantity like the total energy).