Furthermore, the computed and experimental results are only partially comparable because of the difference in the relevant temperatures. Thus, it seems reasonable to assume that the computed transition does, in fact, represent the observed isomorphic phase transition in cesium, thereby providing justification for the assumptions of Yamashita and Asano [10] and Kmetko [11].

The APW wave functions are expanded, in each sphere, in spherical harmonics, which allows the charge of each state to be broken down, inside the spheres, into components associated with each value of ℓ in the spherical harmonic expansion [2]. The sums over all occupied valence states of these components is indicative of, though not identical to, the contributions of the corresponding atomic states to the occupied valence states in the crystal [4]. These sums together with the amount of valence charge outside the spheres, are plotted for Cs in Fig. 3 as a function of lattice volume per atom. The behavior of the d-like (ℓ=2) part of the valence charge reveals an interesting extension of Sternheimer's [9] hypothesis regarding the nature of the isomorphic phase transition: even though the d-bands are broad, the transition appears to be intimately associated with a sharp increase in the d-like character of the fcc valence charge, as the lattice volume is decreased. This increase (at about 400 c.a.u.) is clearly associated with the dip in the pressure curve which occurs at the

same atomic volume. Furthermore, the structure (fcc or bcc) which has more d-like charge at any volume also has the lower computed pressure at that volume. Even the topological changes which occur in the Fermi surface can be closely correlated with the kinks in the curve of this d-like charge component [16]. Thus, Sternheimer's explanation appears to have a very great deal of truth, if slightly generalized to allow for broader d-bands.