respect to the Xα one-electron orbitals [6]. The prescription gives α to be 0.69941 for Cs, 0.715 for V, 0.7165 for Ti, and 0.7581 for C. α = 2/3 was used between (outside) the spheres for TiC. For NbC, α = 1 was used everywhere, as originally suggested by Slater [7]. The results presented for TiC and NbC should be insensitive to the choice of α, as shown [4] for TiC. The same is true for the cohesive energies, as long as the α-variation is not too great and the same value of α is used in the respective APW spheres as for the isolated atoms (to allow proper cancellation of terms arising from the core electrons). The magnetization curve calculated for V may show somewhat more dependence on α, though this has not been computationally verified; the form of the curve is expected to be insensitive to α, however.

CESIUM

Cesium metal undergoes a phase transition from bcc to fcc structure at 23 kbar. At 42 kbar it experiences another phase transition, often called isomorphic, in which its unit cell volume decreases by about 9% without change of crystal structure [8]. Sternheimer [9], in 1949, concluded that the isomorphic transition is due to the crossing of the previously unoccupied 5d bands through the partially occupied 6s band as the lattice constant is decreased. More recent calculations by Yamashita and Asano [10] and by Kmetko [11] have shown that the cesium d-bands are broader than those obtained by Sternheimer, indicating that his explanation may be an oversimplification. These calculations have also shown some very interesting topological changes in the Fermi surface which are computed to occur in the range of unit-cell volume across which the phase change occurs. However, they have not included the estimates of cohesive energy, pressure, and enthalpy necessary to determine if the computed electronic properties do, in fact, give rise to a phase transition. Since the Fermiology of Cs has not been experimentally studied at the very high pressures at which the transition takes place, there has been no conclusive evidence that the calculated effects actually correspond