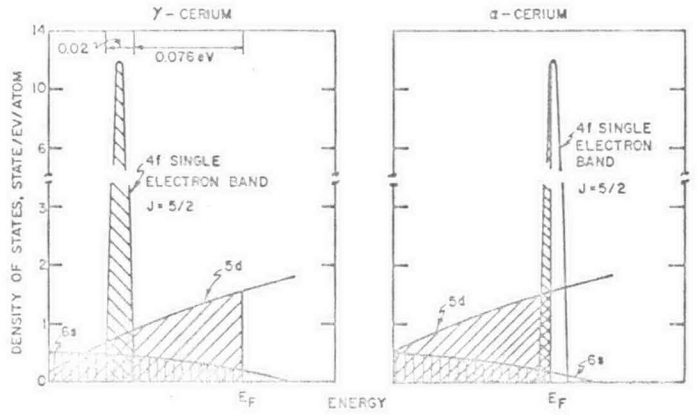

Fig. 6. Band structure of γ-Ce (a) and α-Ce (b).

lengths, which are probably due to intra-atomic transitions from the J = 5/2 (ground state) multiplet to the J = 7/2 multiplet. [35] The above model for cerium, however, is not capable of explaining this 15.5 μ absorption peak.

A model which is capable of explaining this and most of the observed physical properties is shown in Fig. 6a. The 15.5μ absorption would be due to the excitation of electrons from the narrow 4f single electron band to the 5d or 6s band at the Fermi level. The wavelength at which this transition occurs, suggests that the 4f level lies 0.076 eV below the Fermi energy and the width of the transition suggests that the one electron 4f band is very narrow, about 0.02 eV wide. The height of the 4f band is not known, but it is assumed to be higher than the density of states value obtained from the electronic specific heat constant of α-Ce (see Section 7.2). The Boltzmann distribution (exp $\Delta E/k$ T) indicates that at room temperature 0.05 electrons are thermally excited to the 5d 6s band. This means that γ-Ce has an effective valence of 3.05, which is in very good agreement (better than one might expect) with the valence proposed by Gschneidner and Smoluchowski [3]. Since these authors based their valence on the magnetic properties and the atomic size of γ-Ce, these properties fit this model. Furthermore, since the

height of the 5d band at the Fermi level and the number of holes in the 6s band were derived from the specific heat and the Hall coefficient data, respectively, these properties naturally are in agreement with this model.

Rocher [29] suggested that a virtual 4f bound state model could explain the behavior of cerium (presumably γ-Ce) at high temperatures. In order to explain the high resistivity and the magnetic susceptibilities of cerium he proposed that cerium had a very large density of states (implying a partially occupied 4f band), which he believed was confirmed by the low temperature specific heat data of Parkinson and Roberts. [36] This, however, leads to two difficulties: (1) the low temperature specific heat data which yield a large γ value are appropriate for α-Ce and not γ-Ce* and (2) this large value of γ gives a C_v^e contribution at 300°K of 1.26 cal/g-at. deg and leads to a Debye temperature of 500°K, which is a factor of two to three times larger than those of any of the other rare earth metals. Furthermore, this model does not explain the large infrared absorption at 15.5μ. For these reasons it is felt that the virtual 4f bound state model does not apply to γ-Ce, however, it may be a valid model for α-Ce (see below).

Rocher [29] also pointed out that a large value of the density of states is required to explain the magnetic contribution to the resistivity and the high temperature magnetic susceptibility of γ-Ce. If this is correct, then this casts some doubt on the validity of the band model proposed herein for γ-Ce.

Rocher [29] gives a value of 70 μ ohm-cm for magnetic resistivity of cerium. This value is unreasonably large. Recent resistivity values for lanthanum vary from 57 to 80 μ ohm-cm [38, 39, 40] and for cerium from about 75 to 85 μ ohm-cm [38, 39]. If cerium had a magnetic resistivity of about 70 μ ohm-cm as suggested by Rocher, we would expect cerium to have a room temperature resistivity of 125 to 150 μ ohm-cm (*i.e.* about 70 μ ohm-cm larger than that of lan-

* At temperatures below 100°K all of the γ-Ce has transformed to α-Ce. [37]