α - BCT - HCP transition in CE from first principles

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We have studied the lattice dynamics of the α and γ Ce phases, using pseudopotential calculations within the density functional theory. We find that the theoretical phonon spectrum of the low-density Ce phase at ambient pressures is in good agreement with the experimental neutron scattering data. Upon transition to the higher density phase, we find anomalous behaviour of the transverse acoustic branch along the [110] direction, the slope of which at γ, corresponds to the C' elastic constant. We further find the softening of this branch close to γ point, to be responsible for the structural transformation to the bct phase upon pressure. Experimentally, the Ce phase diagram along the pressure axis is complicated by the observation of several intermediate phases at lower pressures. We are able to establish the nature of these phases, by studying the phonon instabilities of the bct phase at these pressures. Furthermore we study in detail a martensitic transition path from bct to hcp at higher pressures. In conclusion, we find that the complicated phase diagram of Ce can be described in terms of intermediate stable structures on a martensitic transformation path between fcc and hcp.