Charge ordering as alternative to Jahn-Teller distortion

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It was pointed out in the seminal paper of Jahn and Teller that a partially occupied degenerate molecular level, often a doubly degenerate E_g level in a cubic ligand field, is unstable against a distortion that splits the level and lowers the total energy of the occupied states. Since then, this effect has been commonly found in solids where it takes a form of a *cooperative* Jahn-Teller (JT) effect (orbital ordering), when the crystal lattice distorts coherently so as to lift orbital degeneracy at each site or, in band language, to split an entire band (*e.g.*, e_g) and thus open a gap at the Fermi level. Upon the gradual delocalization of degenerate electrons, the JT distortion and corresponding orbital ordering becomes less and less favorable, but, as we show, below a crossover region exists with the possibility of lifting degeneracy not by an *orbital ordering*, but by a *charge ordering* (CO): an electron can be transferred from one ion to another, so that, say, the doubly degenerate e_g level on one site will be fully occupied, and on the other site empty. In this paper we demonstrate, experimentally and by first principles calculations, that just such a "JTCO" effect actually occurs in the rare earth nickelates such as $YNiO_3$ and $LuNiO_3$. Apparently this novel phenomenon can also take place in other similar systems.