



## Glenn T. Seaborg Center Seminar

### Cerocene: A Molecule that Brings Tears to my Heart

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Wednesday, 26 September 2007, 4:00–5:00pm, 70A-3377

Cerocene,  $\text{Ce}(\text{C}_8\text{H}_8)_2$ , prepared forty years ago(1), was assumed to be isostructural with the more celebrated uranocene and thorocene analogues, all of which have  $D_{8h}$  symmetry. This proposition was shown to be correct only recently (2). The electronic structure of cerocene was assumed to be identical to that of thorocene, a deduction that is consistent with their identical photoelectron spectra (3). Early molecular orbital calculations made the outrageous conjecture that the electronic structure of cerocene is  $\text{Ce}(\text{III}, f^1)(\text{cot}^{-1.5})_2$  with an  $^1A_{1g}$  ground state and it is a "molecular analogue of a Kondo singlet state" (4). This proposition was supported and extended by CI-calculations, which claimed that the ground state is an admixture of the two states,  $\text{Ce}(\text{III}, f^1)(\text{cot}^{-1.5})_2(e_{2u}^3)$  and  $\text{Ce}(\text{IV}, f^0)(\text{cot}^{-2})_2$  in an approximate ratio of 80:20 (5). Thus, the ground state is multi-configurational and non-magnetic since the former state is an open-shell singlet. The seminar will outline the evolution of these concepts, the synthesis details for preparing cerocene in quantity and in pure form, and experimental measurements of the magnetic susceptibility and XANES data, which support the CI-calculations that cerocene really is a Kondo singlet molecule(6).

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