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(Summary in English)

Metallocenes constitute a prototypic group of metalloorganic compounds. The discovery of ferrocene indicated the intensive development of metalloorganic chemistry. The recently revealed new high-pressure crystal phase I' and modulated phase I'' of ferrocene convinced me to investigate also other prototypic metallocenes. The structural analysis of nickelocene and ferrocene, by applying the model of independent rotation of cyclopentadienyl rings to their isostructural phases I, shows that the staggered molecular conformation coexists with rotated conformations. Based on structural data, this 'soft model' explains the previously reported dielectric properties of ferrocene. These properties were inconsistent with the C_5 symmetry of ferrocene molecules.

The compression of α -ruthenocene (α -RuCp₂, space group *Pnma*) and α -osmocene (α -OsCp₂, *Pnma*) crystals lead to phase transitions, which change of crystal symmetry into space group *Pcmb* (β -RuCp₂) and *Pcab* (β -OsCp₂). The Raman spectra, diffractometric measurements on powder samples, and visual observations of single crystals revealed a wide hysteresis of the $\alpha - \beta$ phase transitions between 0.7-3.9 GPa (RuCp₂) and 0.3-3.6 GPa (OsCp₂). The high-pressure β polymorphs are stabilized by short contact CH \cdots M ($M = \text{Ru, Os}$), whereas phase α is dominated by bonds CH \cdots π . Diffractometric measurements on single crystals of RuCp₂ and OsCp₂ at ambient pressure and 395 K and 427 K respectively reveal the α to γ phase transitions. The high-temperature γ phases are isostructural, space group *Fmmm*. These phase transitions break all CH \cdots M bonds, and the molecules become disordered in staggered and eclipsed conformations.