Poster

Competition between CH···π and CH···M contacts in metallocenes structures

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Ferrocene ($FeCp_2$), [1] ruthenocene ($RuCp_2$) [2] and osmocene ($OsCp_2$) [3] are the only known simple metallocenes, which crystallize in orthorhombic system with eclipsed conformation of cyclopentadienyl rings. The structures at 0.1 MPa/ 296 K of $RuCp_2$ (α-$RuCp_2$) and $OsCp_2$ (α-$OsCp_2$) and low-temperature phase of $FeCp_2$ are isostructural (space group *Pnma*) and mostly stabilize by CH···π contacts. We also discovered a new high-pressure phase of $RuCp_2$ (β-$RuCp_2$) [4] and $OsCp_2$ (β-$OsCp_2$) [5] which differ from each other. In spite of differences in crystal symmetry of β-$RuCp_2$ and β-$OsCp_2$, the reason of occurring phase transitions was the same - higher preference to CH···M bond creations at high-pressure conditions. In β-$RuCp_2$ (space group *Pcmb*) one ruthenocene molecule creates only one close CH···M contact, while in β-$OsCp_2$ (space group *Pcab*) there are four symmetry independent CH···M contacts per one molecule (Fig. 1).

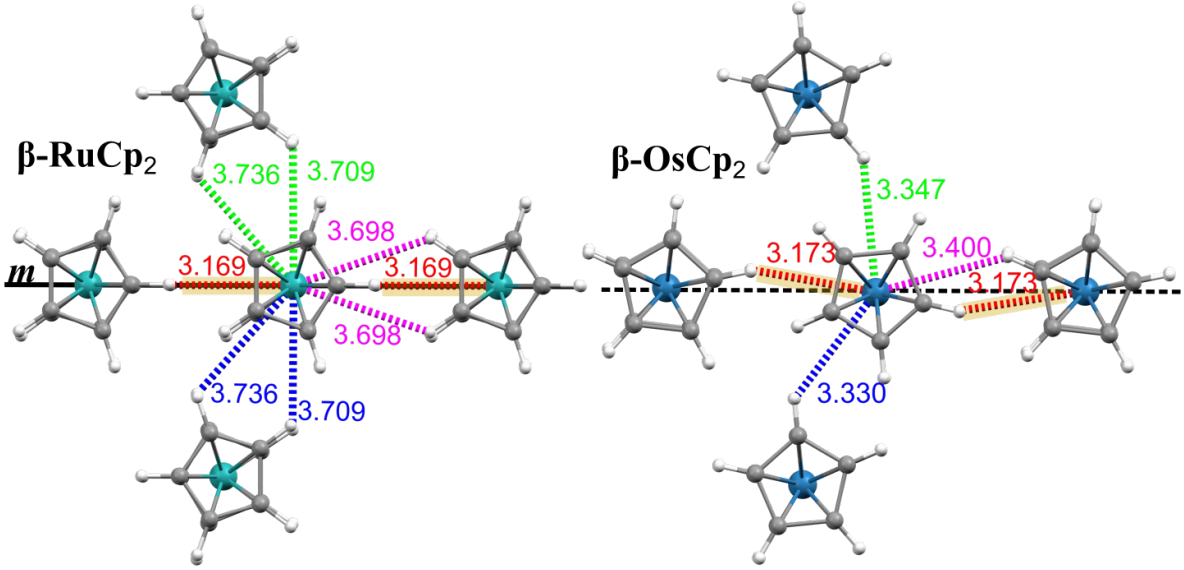

Figure 1. CH···M bonds in β-$RuCp_2$ at 1.00 GPa and in β-$OsCp_2$ at 1.05 GPa. The interacting molecules are viewed along their axes, lying in the mirror planes for ruthenocene and close to glide plane *a* for osmocene. The indicated distances are given in angstroms.

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