

VORTRAG IM RAHMEN DES SONDERFORSCHUNGSBEREICHS 623
DER UNIVERSITÄT HEIDELBERG
MOLEKULARE KATALYSATOREN: STRUKTUR UND FUNKTIONSDESIGN

Freitag, 30.07. 2004, 11 Uhr c. t.

Kleiner Hörsaal, Im Neuenheimer Feld 252

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“C-C bond formation reactions promoted by CpRuX fragments: a DFT study

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A complete catalytic cycle for the cyclotrimerization of acetylene with the CpRuCl fragment is proposed based on DFT/B3LYP calculations. The first intermediate is a metallacyclopentatriene complex $\text{RuCp}(\text{Cl})(\text{C}_4\text{H}_4)$, generated through oxidative coupling of two alkyne ligands. It adds another alkyne in η^2 fashion. Three successive intermediates could be located: an unusual five and four-membered bicyclic ring system (**D**), which rearranges to a very unsymmetrical metallaheptatetraene complex (**E**), and leads to $\text{CpRuCl}(\eta^2\text{-C}_6\text{H}_6)$ (**F**) via a reductive elimination step. Possible pathways connecting the metallacyclic derivative of RuCpX ($\text{X} = \text{Co}$ or PH_3) with a isomeric cyclobutadiene complex are also explored. DFT/B3LYP calculations were used to support the proposed pathway.”

Gäste sind herzlich willkommen.

Bei Interesse an einem Gesprächstermin bitte melden bei Frau Windisch in der
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DER SPRECHER
gez. P. Hofmann