DFT Calculations on m-Vinylidene Titanium-Gold Complexes

Uwe Böhme[a], Rüdiger Beckhaus[b]

[a] Institut für Anorganische Chemie, Leipziger Straße 29, Technische Chemie Universität Bergakademie Freiberg, D-09596 Freiberg, Germany

[b] Fachbereich Chemie, Carl von Ossietzky Universität Oldenburg, D-26111 Oldenburg, Germany

In the course of investigations concerning the vinylidene intermediate [Cp_2*Ti=C=CH_2] [1] we were interested in the structure and bonding situation of heterobinuclear vinylidene-bridged complexes. The X-ray structure analysis of the titanium-gold complex Cp*$_2$Ti(Cl) (m-vinylidene) $AuPPh_3$ shows an asymmetrically bridged m-vinylidene structure with trigonal-planar coordination of the gold atom. [2]

Quantum chemical calculations at the DFT level of theory (B3LYP) in conjunction with effective core potentials and different valence basis sets are reported for the model complexes Cl-Au-PR_3 and Cp_2Ti(Cl)(m-vinylidene)$AuPR_3$ (R=H, Me). The calculated geometries are compared with data from X-ray structure analyses and the nature of the binding interactions has been analyzed with the help of the NBO partitioning scheme.

[1] R. Beckhaus , Angew. Chem. 109 (1997) 694-722 ; Angew. Chem. Int. Ed. Engl. 36 (1997) 686-713. - R. Beckhaus , J. Chem. Soc., Dalton Trans. (1997) 1991-2001.

[2] R. Beckhaus, J. Oster, R. Wang and U. Böhme, Organometallics 17 (1998) 2215-2221.