The Agostic interaction in transition metal and actinide methylidene complexes

Björn O. Roos Department of Theoretical Chemistry Chemical Center, University of Lund P.O. Box 124, S-221 00 Lund, Sweden

Abstract

The lecture will discuss the agostic interaction that takes place between the methylene hydrogen and the metal in complexes of the type H₂MCH₂, where M is a transition metal or an actinide. CASSCF/CASPT2 optimizations of the geometry have been performed for a number of such complexes. The analysis is made in terms of the natural orbitals and other properties of these compounds.