

Supplementary Data

Is the C-Mo Bond in a Small Molybdenum Methylidyne Really a Triple Bond?

Han-Gook Cho

Department of Chemistry, University of Incheon, Incheon 406-772, Korea. *E-mail: hgc@incheon.ac.kr
Received January 22, 2011, Accepted May 25, 2011

Key Words : Carbon-molybdenum bond, Bond order, Methylidyne, CASSCF, NBO

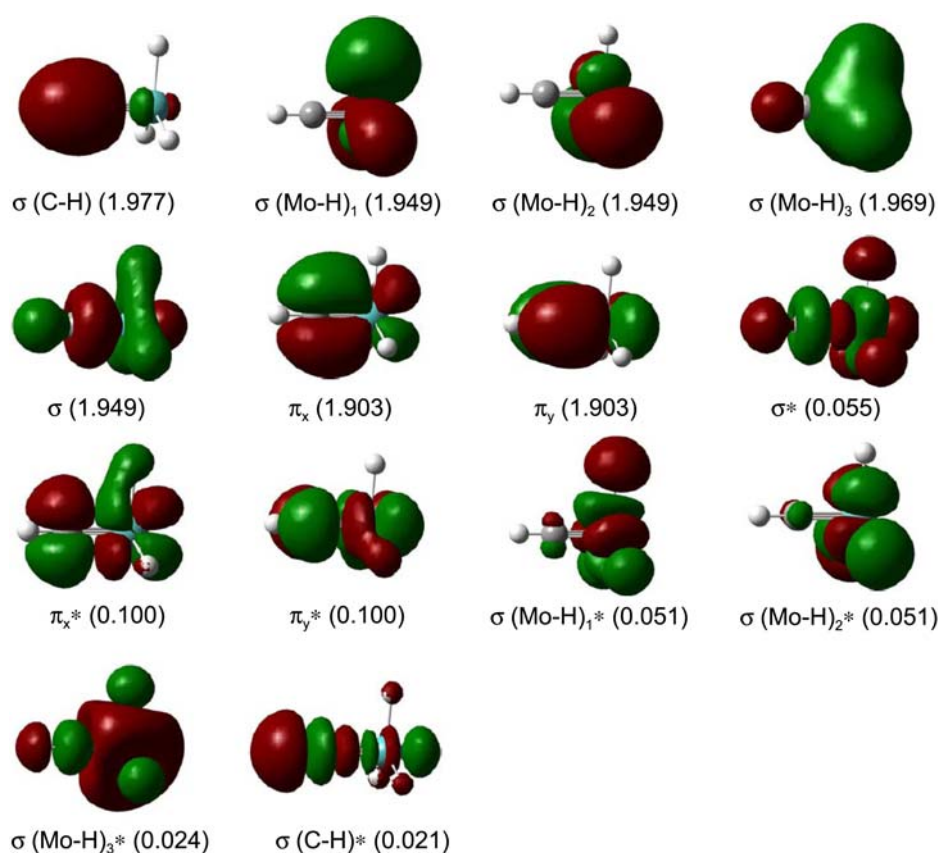


Figure S1. Calculated CAS(14,14) orbitals involved in the carbon-molybdenum triple bond. Occupation numbers are given in parentheses, and the effective bond order (EBO) = 2.750, showing only a slight change from that of CAS(6,6).