Calculated geometry and paramagnetic hyperfine structure of the Cu7 cluster

Arratia-Pérez, Ramiro

Alvarez-Thon, Luis

Fuentealba, Patricio

All-electron spin polarized DFT calculations have been performed to optimize the pentagonal bipyramidal (D5h) geometry of the Cu7 cluster by using the B3LYP and the B3PW1 functionals with different basis sets. Dirac scattered-wave and its non-relativistic limit calculations are used to calculate the 63Cu hyperfine coupling constants using a first order perturbational procedure. Our calculations for the Cu7 cluster predict the 2 A2? as its ground state. The calculated hyperfine coupling constants are in reasonable agreement with those experimentally determined for Cu7 in a matrix isolated ESR study by Van Zee and Weltner [J. Chem. Phys. 92 (1990) 6976].