Theoretical study of electronic spectra of [Pt3(?-CO) 3(CO)3]n-2 (n = 3-5) complexes

Mendizabal, Fernando

Burgos, Darwin

Olea-Azar, Claudio

The platinum-platinum attraction and the spectroscopic properties of [Pt3(?-CO)3(CO)3]n-2 (n = 3-5) were studied at the PBE level. Theoretical calculations are in agreement with experimental geometries. The absorption spectra of these platinum complexes were calculated by the single excitation time-dependent (TD) density functional method. All complexes showed MLCT transitions interrelated with the intertriangular complexes. The values obtained at the PBE level are in agreement with the experimental color range.