# Theoretical study on electronic spectra and aurophilic attraction in [Au3 (MeN {double bond, long} COMe)3]n (n = 1 s(-) 4) complexes

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The aurophilic attraction and the spectroscopic properties of [Au3 (MeN {double bond, long} COMe)3]n (n = 1 s(-) 4) were studied at the MP2 and density functional theory (B3LYP and PBE) levels. Theoretical calculations at the MP2 level are in agreement with experimental geometries and aurophilic attraction, and to a lower extent for PBE. The absorption spectra of these gold(I) complexes were calculated by the single-excitation time-dependent (TD) density functional method. All complexes showed MMCT and MLCT transitions interrelated with the gold-gold intermolecular distance. The values obtained at the PBE level are in agreement with the experimental range. 