

# Theoretical study of $\{Au_3(CH_3NCOCH_3)_3\}_n \cdot \{2,4,7\text{-trinitro-9-}\mu\text{urenone}\}$ ( $n = 1,2$ ) complexes

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The interaction between  $Au_3(CH_3NCOCH_3)_3$  and  $\{2,4,7\text{-trinitro-9-}\mu\text{urenone}\}$  and the electronic structure and spectroscopic properties of  $\{Au_3(CH_3NCOCH_3)_3\}_n \cdot \{2,4,7\text{-trinitro-9-}\mu\text{urenone}\}$  ( $n = 1,2$ ) are studied at the HF, MP2, and PBE levels. Secondary  $\pi$ -interactions ( $Au$ - $\mu\text{urenone}$ ) were found to be the main contribution to short-range stability in the  $\{Au_3(CH_3NCOCH_3)_3\}_n \cdot \{2,4,7\text{-trinitro-9-}\mu\text{urenone}\}$  complex. At the MP2 and PBE levels, Au-C equilibrium distances of 292.3 and 304.0 pm and interaction energies of 105.3 and 24.9 kJ/mol were found, respectively. The absorption spectra of these complexes were calculated by the single excitation time-dependent method at the PBE level. The theoretical values obtained are in agreement with the experimental range. © 2009 Wiley Periodicals, Inc.