Theoretical study on interactions of fluorinated organomercurials with arene and gold fragments

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The electronic structure and spectroscopic properties of [Hg(C<inf>6</inf>F<inf>5</inf>)<inf>2</inf>]<inf>2</inf>-{L}, [Hg<inf>3</inf>(o-C<inf>6</inf>F<inf>4</inf>)<inf>3</inf>]<inf>2</inf>·{L} (L = naphthalene, biphenyl, fluorene) and [Hg<inf>3</inf>(o-C<inf>6</inf>F<inf>4</inf>)<inf>3</inf>]{Au<inf>3</inf>(?-C(OEt)=NC<inf>6</inf>H<inf>4</inf>CH<inf>3</inf>)<inf>3</inf>}<inf>n</inf> (n = 1, 2) adducts were studied at the HF, MP2, SCS-MP2, DFT and DFT-D3 levels. The intermolecular interactions among the fragments were analyzed using the levels of calculations proposed. The energy decomposition analysis at the TPSS-D3 level was used to define the dominant components of the interaction. The van der Waals interactions between mercury and arene (Hg-arene) were found to be the main short-range stability contribution in the [Hg(C<inf>6</inf>F<inf>5</inf>)<inf>2</inf>]<inf>2</inf>-{L} and [Hg<inf>3</inf>(o-C<inf>6</inf>F<inf>4</inf>)<inf>3</inf>]<inf>2</i