A comparative study between post-Hartree-Fock methods and density functional theory in closed-shell aurophilic attraction

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The inter- and intramolecular aurophilic [ClAuPH3]2, [S(AuPH3)2] and [AuPH3]42+ interactions were studied using ab initio post-Hartree-Fock and DFT methodologies. The post-Hartree-Fock methods provide results closer to the experimental data than DFT-based methods. It is possible to highlight the results obtained by the SCS-MP2 and CCSD(T) methods. In the classic [ClAuPH3]2 dimer, the aurophilic interaction is driven by the induction and dispersion terms. When DFT is used, the best results of geometry and interaction energy are obtained with the PW91 level. We find -D3 Grimme correction, M06HF, M06L, M06 M062X, M052X, CAM-B3LYP and LC-?PBE provided results of similar accuracy as MP2.