

# Theoretical study of the d10-s2 interaction between Au(I) and Tl(I) in the [AuCl(PH<sub>3</sub>)<sub>2</sub>]<sup>+</sup>Tl<sup>+</sup> hypothetical complex

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We studied the attraction between Au and Tl in the [AuCl(PH<sub>3</sub>)<sub>2</sub>]<sup>+</sup>Tl<sup>+</sup> complex using ab initio methodology. This is a hypothetical compound. We found that the changes around the Au-Tl equilibrium distance and in the interaction energies are sensitive to the electron correlation potential. This effect was evaluated using HF, MP2, MP4 and CCSD(T) levels. The obtained interaction energy differences in the equilibrium distance (Au-Tl) ranged from 37 to 98 kJ/mol. At long distances, the behaviour of the [AuCl(PH<sub>3</sub>)<sub>2</sub>]-Tl<sup>+</sup> interaction may be mainly related to charge-induced dipole and dispersion terms. The charge-induced dipole term was found to be principally contributing to the stability. The dispersion interaction was smaller, but not negligible. © 2009 Elsevier B.V. All rights reserved.