Theoretical study of the interaction between Au(I) and I on the [AuI2]--I2 complexes

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We studied the interaction between [AuI2]- and I2 using ab initio methodology. We found that the changes around the equilibrium intermolecular distance Au...I2 and in the interaction energy differences are sensitive to the electron correlation potential. We evaluated these effects using several levels of theory, including MP2, MP4 and CCSD(T); and size of the basis set on atoms. The equilibrium distances Au-I2 in the complexes are in the range 380-392pm. The obtained interaction energies differences at the equilibrium distance range from 4.3 to 14.7kJ/mol at the different levels used. These results indicate that the complexes formed are in the category of van der Waals systems. At long-distances, the behaviour of the [AuI2]-...I2 interaction may be related mainly to charge-induced dipole and dispersion terms. Both terms are important.