The Smallest “Aurophilic Species”

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The existence of the \( C_{2v} \) symmetric closed-shell di\[gold(I)\]hydronium cation \([Au_2H]^+\) (1), is predicted. It is shown that 1 is the smallest possible molecular species containing aurophilic contacts. Equilibrium structural parameters, vibrational frequencies and formation energies of 1 from \( Au^+ \) and \( AuH \), have been calculated, employing a series of highly correlated but available standard relativistic \textit{ab initio} methods up to CCSD(T) level of theory and all-electron basis sets of quadruple-\( \zeta \) quality with double polarizations. Relativistic effects have been taken into account by employing pseudorelativistic electron core potentials (ECP) or a scalar relativistic treatment using a Douglas-Kroll-Heß Hamiltonian of 2nd, 3rd and 4th order (DKH2, DKH3, DKH4).

Key words: \( \text{Au(I)}-\text{Au(I)} \) Interaction, Metallophilic Interaction, Gold Hydride, Quantum Chemical Calculation