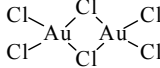
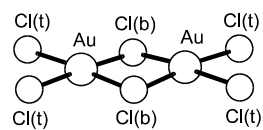


55	Au₂Cl₆	Di-μ-chloro-bis[dichlorogold(III)]	D_{2h}
	ED, <i>ab initio</i> and DFT calculations	Di- μ -chloro-tetrachlorodigold	
	r_g	θ_a	
	Å ^{a)}	deg ^{a)}	
	Au–Cl(t) 2.236(13)	Cl(t)–Au–Cl(t) 92.7(25)	
	Au–Cl(b) 2.355(13)	Cl(b)–Au–Cl(b) 86.8(18)	

The vapor over gold trichloride was found to consist of dimeric gold trichloride molecules (5.8(3) mol%) and all the rest was chlorine gas. Parameters of Cl₂ were taken from the literature and converted to the experimental conditions of this study. The Au₂Cl₆ molecule was found to be planar. According to the explanation by the authors, the distortion of the Jahn-Teller-affected monomer to form a tetrahedral dimer costs a larger amount of energy than to form the planar structure, and the results of B3LYP/aug-cc-pVTZ calculations show that the nonplanar configuration is *ca.* 64 kcal mol^{−1} less stable than the planar form.

The nozzle temperature was 457 K.

^{a)} Estimated total errors.



Hargittai, M., Schulz, A., Réffy, B., Kolonits, M.: J. Am. Chem. Soc. **123** (2001) 1449.