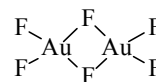


56 **Au₂F₆**ED, *ab initio* and DFT
calculations**Di- μ -fluoro-bis[difluorogold(III)]**Di- μ -fluoro-tetrafluorodigold**D_{2h}**

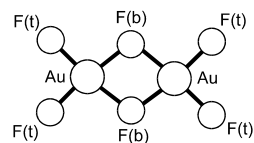
r_g	Å ^{a)}
Au–F(t)	1.876(6)
Au–F(b)	2.033(7)
Au...Au	3.082(6)

θ_a	deg ^{a)}
F(t)–Au–F(t)	92.1(10)
F(b)–Au–F(b)	80.4(16)



The presence of other species, such as the monomeric and trimeric AuF₃ molecules, fluorine or hydrogen fluoride, was tested in the ED analysis and ruled out. The contribution of multiple scattering to the experimental intensities was taken into account. The results indicate that the dimer has a planar F-bridged equilibrium geometry that appears puckered in the ED analysis, as a consequence of the shrinkage effect due to intramolecular vibrations.

The nozzle temperature was 600 K.



^{a)} Estimated total errors.

Réffy, B., Kolonits, M., Schulz, A., Klapötke, T.M., Hargittai, M.: J. Am. Chem. Soc. **122** (2000) 3127.