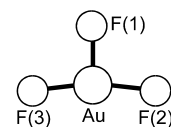


54 AuF₃ED, *ab initio* and DFT
calculations**Gold trifluoride**

Gold(III) fluoride

C_{2v}
AuF₃

r_g	Å ^{a)}	θ_g	deg ^{a)}
Au–F(1)	1.893(12) ^{b)}	F(1)–Au–F(3)	102.5(19)
Au–F(2,3)	1.913(8) ^{b) c)}	F(2)–Au–F(3)	160.4(41)



The molecule was found to exist as a mixture of monomeric (94.4(40)%) and dimeric molecules at the nozzle temperature of 1094 K. Both experiment and quantum chemical calculations indicated that the ground-state structure of the molecule has C_{2v} symmetry due to a first-order Jahn-Teller effect. According to the results of CASSCF calculations, the molecule has a typical “Mexican hat”-type potential energy surface with three equal minimum-energy structures around the brim of the hat, separated by equal-height transition structures, about 3.6 kcal mol^{−1}.

^{a)} Estimated total errors.

^{b)} Difference between the Au–F(1) and Au–F(2,3) bond lengths was assumed at the value from B3LYP/basis 2 (Au), aug-cc-pVTZ(F) calculations.

^{c)} Difference between the Au–F(t) in the dimeric molecule and Au–F(2,3) bond lengths was assumed at the value from B3LYP/basis 2 (Au), aug-cc-pVTZ(F) calculations.

Réffy, B., Kolonits, M., Schulz, A., Klapötke, T.M., Hargittai, M.: J. Am. Chem. Soc. **122** (2000) 3127; Erratum: J. Am. Chem. Soc. **123** (2001) 1545.