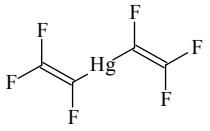
476 **C_4F_6Hg** **Bis(trifluoroethenyl)mercury** **C_2**

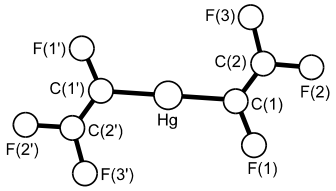
ED, *ab initio* calculations



r_a	Å [a])	θ_a	deg [a])
Hg–C(1)	2.054(3)	C(2)=C(1)–Hg	123.9(7)
C(1)=C(2)	1.326(8)	F(1)–C(1)–Hg	117.9(11)
C(1)–F(1)	1.357(13)	C(2)=C(1)–F(1)	118.2(6)
C(2)–F(2)	1.321(7)	C(1)=C(2)–F(2)	127.0(5)
C(2)–F(3)	1.332(7)	C(1)=C(2)–F(3)	122.7(7)
		F(2)–C(2)–F(3)	110.4(10)

Linearity of the C–Hg–C moiety, planarity of the Hg–CF=CF_2 groups and free rotation of the vinyl groups around the C–Hg–C axis were assumed in the ED analysis. MP2/DZP calculations predicted a shallow potential minimum at the C=C…C=C torsional angle of *ca*. 98.2° with barriers of *ca*. 1.6 and 1.0 kJ mol^{-1} at C_{2v} and C_{2h} forms, respectively. The nozzle temperature was *ca*. 361 K.

[a]) Estimated standard errors.



Banger, K.K., Brisdon, A.K., Brain, P.T., Parsons, S., Rankin, D.W.H., Robertson, H.E., Smart, B.A., Bühl, M.: Inorg. Chem. **38** (1999) 5894.