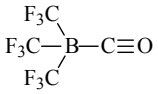
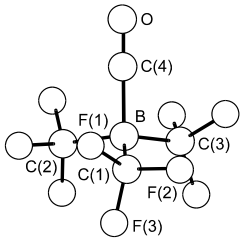
472 **C_4BF_9O** **Carbonyltris(trifluoromethyl)boron** **C_3** assumed

ED, MW, *ab initio* and DFT calculations



r_{h1} [a])	Å [b])	θ_{h1} [a])	deg [b])
C≡O	1.124 [c])	C(4)–B–C(1)	103.8(4)
C(4)–B	1.617(12)	C(1)–B–C(2)	114.5(4)
C(1)–B	1.631(4)	F(1)–C(1)–F(2)	107.2(1)
C(1)–F(1)	1.358(1) [d])	tilt(CF_3) [e])	0.8 [f])
C(1)–F(2)	1.348(1) [d])	τ [g])	11.5(9)
C(1)–F(3)	1.337(1) [d])		



The nozzle was at room temperature.

[a]) Nonlinear kinematic effects were taken into account.
[b]) Twice the estimated standard errors.
[c]) Estimated using the r_0 distance for CO molecule from the literature.
[d]) Differences in the C–F bond lengths were assumed at the values from MP2/cc-pVDZ calculations.
[e]) Tilt angle of the CF_3 group, which makes the B–C(1)–F(2) angle larger than the B–C(1)–F(3) and B–C(1)–F(1) angles.
[f]) Assumed at the value from HF/6-311G(2d) calculations.
[g]) C(4)–B–C(1)–F(3) torsional angle, $\tau = 0°$ for the *anti* position.

Finze, M., Bernhardt, E., Terheiden, A., Berkei, M., Willner, H., Christen, D., Oberhammer, H., Aubke, F.: J. Am. Chem. Soc. **124** (2002) 15385.