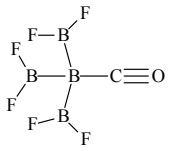
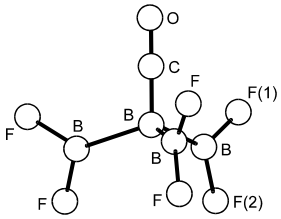
11 **CB_4F_6O** **Carbonyltris(difluoroboryl)boron** essentially C_{3v}

ED, *ab initio* and DFT calculations



r_a	Å [a])	θ_a	deg [a])
O≡C	1.158(3)	C–B–B	108.3(24)
C–B	1.502(5)	B–B–F [b])	122.2(6)
B–B	1.694(3)	Δ(B–B–F) [c])	2.6(1) [d])
B–F [b])	1.330(1)	C–B–B–F	2.0(2) [d])
Δ(B–F) [e])	0.015(1)		



The $B–BF_2$ groups were assumed to be planar.
The nozzle temperature was 298 K.

[a]) Estimated standard errors.
[b]) Mean value.
[c]) [B–B–F(1)] – [B–B–F(2)].
[d]) Restrained to the value from MP2/6-311G* calculations.
[e]) [B–F(1)] – [B–F(2)].

Mackie, I.D., Hinchley, S.L., Robertson, H.E., Rankin, D.W.H., Pardoe, J.A.J., Timms, P.L.: J. Chem. Soc., Dalton Trans. (2002) 4162.