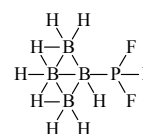


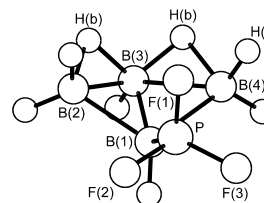
72 B₄F₃H₈PED, *ab initio*
calculations**1-(Trifluorophosphine)-*arachno*-
tetraborane(10)**

1-(Phosphorous trifluoride)tetraborane(8)

C_s assumed (*endo*)

r_{α}^0	Å ^{a)}	θ_{α}^0	deg ^{a)}
B(1)–B(3)	1.722(12)	B(3)–B(1)–P	131.6(11)
B(1)–B(2)	1.847(9)	P–B(1)–H	108.5(18)
B(2)–B(3)	1.799(10)	B(1)–B(3)–H	115.0 ^{b)}
B(1)–P	1.798(9)	F–P–F ^{c)}	100.2(1)
P–F(1)	1.522(1) ^{d)}	ϕ ^{e)}	133.9(23)
P–F(2,3)	1.530(1) ^{d)}	τ ^{f)}	180.0 ^{b)}
B(3)–H(b)	1.307(16)	tilt(PF ₃) ^{g)}	–3.5(11)
B(4)–H(b)	1.365(18)		
B–H(t) ^{h)}	1.200(9)		

According to MP2/TZP calculations, the *exo* isomer lies 9.3 kJ mol^{–1} higher than the *endo* form, corresponding to an *endo:exo* ratio of *ca.* 98:2 at room temperature. The experimental data were fitted using a model of the *endo* isomer. Differences in the B–B and B–H distances were constrained to the values from MP2/6-31G* calculations. The presence of impurity (carbonyltetraborane(8), B₄H₈CO (3.5%)) was taken into account. The nozzle temperature was about 296 K.

^{a)} Estimated standard errors.^{b)} Assumed.^{c)} All the F–P–F angles were assumed to be equal.^{d)} Difference between the P–F(1) and P–F(2,3) distances was assumed at the value from MP2/6-31G* calculations.^{e)} Angle between the B(1)B(2)B(3) and B(1)B(3)B(4) planes.^{f)} H–B(1)–P–F(1) torsional angle from the *syn* position.^{g)} Angle between the C₃ axis of the PF₃ group and the B(1)–P axis, positive value when the PF₃ group is tilted away from the inside of the “butterfly”.^{h)} Mean value.

Brain, P.T., Rankin, D.W.H., Robertson, H.E., Fox, M.A., Greatrex, R., Nikrahi, A., Bühl, M.: *Inorg. Chem.* **36** (1997) 1048.