

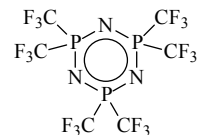
693 **C₆F₁₈N₃P₃**
ED, *ab initio* and DFT
calculations

**2,2,4,4,6,6-Hexahydro-2,2,4,4,6,6-hexakis-
(trifluoromethyl)-1,3,5,2,4,6-triazatriphosphorine**
Hexakis(trifluoromethyl)cyclotriphosphazene

D_{3h} assumed

r_a	\AA^a
P–N	1.583(3)
P–C	1.870(2)
C–F	1.333(1)

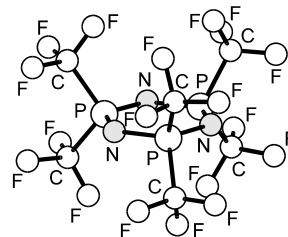
θ_a	deg ^{a)}
N–P–N	119.5(7)
P–N–P	120.5(7)
C–P–C	105.5(12)
F–C–F	108.6(7)
tilt(CF ₃) ^{b)}	0.6(15)



Local C_{3v} symmetry was assumed for the CF₃ group.
The nozzle was at room temperature.

^{a)} Three times the estimated standard errors.

^{b)} Tilt angle between the C₃ axis of the CF₃ group and P–C bond direction away from the opposite CF₃ group.



Trautner, F., Singh, R.P., Kirchmeier, R.L., Shreeve, J.M., Oberhammer, H.: *Inorg. Chem.* **39** (2000) 5398.