

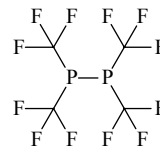
481 **C₄F₁₂P₂**ED, *ab initio*
calculations**Tetrakis(trifluoromethyl)diphosphine**

Tetrakis(trifluoromethyl)diphosphane

C_{2h} assumed (*anti*)**C₂ assumed (*gauche*)**

r_a	\AA^a
P–P	2.248(11)
P–C	1.896(4)
C–F	1.337(2)

θ_a	deg ^{a)}
P–P–C	96.2(10)
C–P–C	98.8(28)
F–C–F	107.4(2)
tilt(CF ₃) ^{b)}	4.2(12)
τ^c	–174.8(41)



The molecule was found to exist as a mixture of *anti* (85(10)%) and *gauche* conformers.

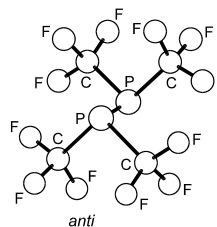
Local C_{3v} symmetry was assumed for CF₃ groups. The molecular parameters of both conformers were assumed to be equal except for the P–P–C angles and the torsional angles. The differences between the P–P–C angles were assumed at the values from HF/6-311+G* calculations. The parameters are listed for the *anti* conformer.

The nozzle was at room temperature.

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

^{b)} Angle between the C₃ axis of the CF₃ group and the P–C vector towards the lone pair of the P atom.

^{c)} C–P–C–F torsional angle, $\tau = 0^\circ$ for the *syn* position.



Becker, G., Golla, W., Grobe, J., Klinkhammer, K.W., Le Van, D., Maulitz, A.H., Mundt, O., Oberhammer, H., Sachs, M.: Inorg. Chem. **38** (1999) 1099.

Replaces [II/25C \(3, 1488\)](#)