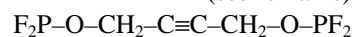


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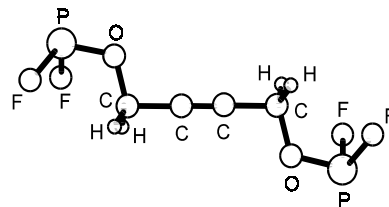
C₄H₄F₄O₂P₂

1,4-Bis(difluorophosphinoxy)-2-butyne

essentially C_{2h}
(see remarks)



r_a	Å ^{a)}	θ_a	deg ^{a)}
P-F	1.598(3)	F-P-F	94.6(11)
P-O	1.553(8)	O-P-F	100.7(8)
C≡C	1.212(14)	C-C-O	105.3(10)
C-C	1.473(16)	C-O-P	118.3(11)
C-O	1.393(15)	C-C-H	109.0 ^{b)}
C-H	1.080 ^{b)}	H-C-H	109.0 ^{b)}
		C-C≡C-C ^{c)}	180 ^{b)}
		P-O-C-C ^{c)}	163.7(16)
		twist (P-O) ^{c)}	1.5(57)



The PF₂O groups are essentially *anti* with respect to each other, though the slight twist about the C-O bond gives C₂ symmetry rather than the C_{2h} symmetry which would otherwise be the case. However, the structure with C_i symmetry was indistinguishable from that with C₂ symmetry. It is probable that torsional vibrations about the C-O bond take the PF₂O groups either side of 180°, and the observed deviation of O-C twist from 180° may be due to shrinkage effects.

The nozzle temperature was 293 K.

^{a)} Estimated standard errors including a systematic error.

^{b)} Assumed.

^{c)} All twist angles are defined to be zero when the point group of the molecule is C_{2v}, the P-O bond is *syn* to C-C and the bisector of F-P-F angle is *syn* to O-C. Each is positive for anticlockwise rotation of the nearer group when viewed along the appropriate bond.

Blake, A.J., Davis, M.J., Rankin, D.W.H.: J. Mol. Struct. **221** (1990) 25.