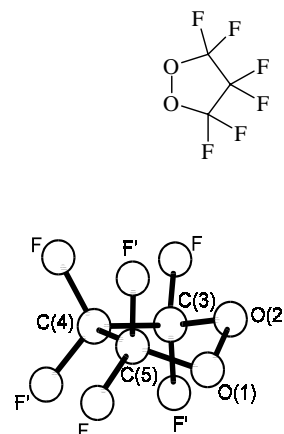


1019 C₃F₆O₂

ED, *ab initio* calculations
(HF/4-21G, HF/4-21G*)

Hexafluoro-1,2-dioxolane
C₂

r_a	Å ^{a)}	θ_α	deg ^{a)}
O–O	1.443(11)	C–C–C	98.1(13)
O–C	1.377(15)	C–C–O	107.3(12)
C–C	1.531(5)	C–O–O	102.9(9)
C–F (mean)	1.318(4)	F–C–F	109.8(9)
$\Delta(\text{C–F})$ ^{b)}	0.010 ^{c)}	rock(F–C(3)–F) ^{d)}	0.0 ^{c)}
C(3)–F	1.315(4)	wag(F–C(3)–F) ^{d)}	2.6 ^{c)}
C(4)–F	1.325(4)	twist(F–C(3)–F) ^{d)}	3.3 ^{c)}
		$\pi(\text{C–O–O–C})$	48(2)
		$\pi(\text{C–C–O–O})$	–38(2)
		$\pi(\text{C–C–C–O})$	15(2)
		q ^{e)}	42(2)



The five-membered ring is in a half-chair conformation. Local C_{2v} symmetry with equal F–C–F angles was assumed for the CF₂ groups.

The nozzle was at room temperature.

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

^{b)} (C(4)–F) – (C(3)–F).

^{c)} Assumed.

^{d)} rock = (1/2)($\alpha_1 - \alpha_2 + \alpha_3 - \alpha_4$); wag = (1/2)($\alpha_1 + \alpha_2 - \alpha_3 - \alpha_4$);
twist = (1/2)($\alpha_1 - \alpha_2 - \alpha_3 + \alpha_4$); $\alpha_1 = \text{C(4)–C(3)–F}$; $\alpha_2 = \text{C(4)–C(3)–F'}$;
 $\alpha_3 = \text{O(2)–C(3)–F}$; $\alpha_4 = \text{O(2)–C(3)–F'}$.

^{e)} Puckering coordinate; for definition see [1].

Jin, A., Mack, H.-G., Waterfeld, A., Dakkouri, M., Oberhammer, H.: J. Mol. Struct. **274** (1992) 163.

[1] Cremer, D., Pople, J.A.: J. Am. Chem. Soc. **97** (1975) 1354, 1358.