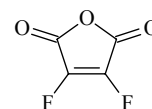


475 **C₄F₂O₃**
ED, MW, *ab initio*
calculations

3,4-Difluoro-2,5-furandione
Difluoromaleic anhydride

C_{2v}



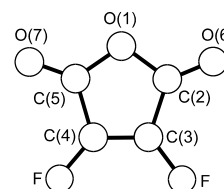
r_a	Å ^{a)}
C(2)=O(6)	1.196(1)
C–F	1.314(2)
C(3)=C(4)	1.336(3)
O(1)–C(2)	1.396(1)
C(2)–C(3)	1.487(3)

r_a^0	Å ^{a)}	θ_a	deg ^{a)}
C(2)=O(6)	1.190(1)	C(2)–C(3)=C(4)	108.3(1)
C–F	1.309(2) ^{b)}	C(4)=C(3)–F	129.9(1)
C(3)=C(4)	1.332(3) ^{b)}	C(3)–C(2)=O(6)	129.3(1)
O(1)–C(2)	1.393(1)	C(2)–O(1)–C(5)	108.9(1)
C(2)–C(3)	1.485(2)	O(1)–C(2)–C(3)	107.2(2)

The nozzle temperature was *ca.* 293 K.

^{a)} Estimated standard errors.

^{b)} Difference between the C–F and C(3)=C(4) bond lengths was refined using flexible restraint estimated according to the results of MP2/6-311+G(2df) calculations.



Abdo, B.T., Amer, H., Banks, R.E., Brain, P.T., Cox, A.P., Dunning, O.J., Murtagh, V., Rankin, D.W.H., Robertson, H.E., Smart, B.A.: J. Phys. Chem. A **103** (1999) 1758.