

Structure Data of Free Polyatomic Molecules

36
ED, IR

CF₂O₂

3,3-Difluorodioxirane

C_{2v}

r_z	Å ^{a)}
C–O	1.348(8)
O–O	1.578(1)
C–F	1.317(6)

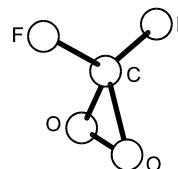
θ_z	deg ^{a)}
F–C–F	108.8(7)
O–C–O	71.7(5) ^{b)}



HF/3-21G and MP2/6-311G(2d) calculations reproduced the experimental bond lengths reasonably well.
The nozzle was at room temperature.

^{a)} Estimated standard errors.

^{b)} Dependent parameter.



Casper, B., Christen, D., Mack, H.-G., Oberhammer, H., Argüello, G.A., Jülicher, B., Kronberg, M., Willner, H.: J. Phys. Chem. **100** (1996) 3983.

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