

Structure Data of Free Polyatomic Molecules

37 **CF₂Se**

MW, IR

Selenocarbonyl fluoride

Carbonoselenoic difluoride

C_{2v}


r_0	Å
C–F	1.3117(1)
C=Se	1.7400(2)

θ_0	deg
F–C–F	107.64(1)

r_z	Å
C–F	1.3123(4)
C=Se	1.7420(5)

θ_z	deg
F–C–F	107.74(4)

r_e^a	Å
C–F	1.309(2)
C=Se	1.739(2)

θ_e^a	deg
F–C–F	107.74(4)

^a) Derived from the r_z structure. r_z was extrapolated to r_e using the relation $r_z = r_e + (3/2)au^2 + K$, where u^2 and K denote the contributions of the mean amplitude and perpendicular amplitude of vibrations, respectively, and a is an anharmonicity parameter that may be estimated by a diatomic model.

Bürger, H., Demaison, J., Dréan, P., Jerzembeck, W., Merke, I., Stahl, W.: Ber. Bunsenges. Phys. Chem. **102** (1998) 872.

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