

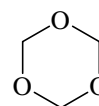
1286
MW

C₃H₆O₃

1,3,5-Trioxane

C_{3v}

r_0	Å	θ_0	deg
C–O	1.422(2)	O–C–O	112.2(2)
		C–O–C	110.3(2)



Colmont, J.M.: J. Mol. Spectrosc. **80** (1980) 166.

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r_a	Å ^{a)}	θ_a	deg ^{a)}
C–O	1.411(2)	O–C–O	111.0(7)
C–H	1.116(11)	C–O–C	109.2(10)
		H–C–H	111.8(37)
		tilt (CH ₂) ^{b)}	0.0 ^{c)}

The nozzle temperature was 80 °C.

^{a)} Estimated standard errors.

^{b)} Angle between an axial C–H bond and the C₃ symmetry axis.

^{c)} Assumed.

Clark, A.H., Hewitt, T.G.: J. Mol. Struct. **9** (1971) 33.