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ED

C₃H₆S₃

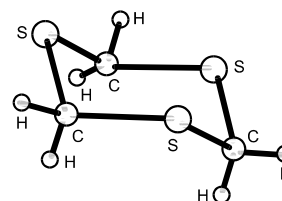
1,3,5-Trithiane

C_{3v}

r_g	\AA^a	θ_a	deg a
S–C	1.812(4)	S–C–S	115.8(1)
C–H	1.114(4)	C–S–C	99.1(4)
		H–C–H	109.7(12)
		ϕ^b	65.2(5)



The experimental data are consistent with the chair conformation of the molecule. The ring is considerably more puckered than that of cyclohexane. The nozzle temperature was ≈ 466 K.



^a) Three times the estimated standard errors.

^b) S–C–S–C dihedral angle.

Bencze, Z., Kucsman, A., Schultz, G., Hargittai, I.: Acta Chem. Scand. **43** (1989) 953.

MW

Structure I ^a):

r_0	\AA^b	θ_0	deg b
S–C	1.815 ^c)	S–C–S	112.4(10)
C–H	1.116 ^c)	C–S–C	103.5(15)
		H–C–H	104 ^c)

Structure II:

r_0	\AA^b	θ_0	deg b
S–C	1.815 ^c)	S–C–S	112.9(10)
C–H	1.095 ^c)	C–S–C	104.4(15)
		H–C–H	109.5 ^c)

^a) The SCS plane is assumed to bisect the H–C–H angle. This probably applies also to structure II.

^b) Uncertainties were not estimated in the original paper.

^c) Assumed.

Cervellati, R., Corbelli, G., Lister, D.G., Alonso, J.L.: J. Mol. Struct. **117** (1984) 247.