

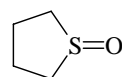
1747
ED

C₄H₈OS

Tetrahydrothiophene 1-oxide

C₁

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(3)–C(4)	1.539(3)	S–C(2)–C(3)	105.3(3)
Δ_1 ^{b)}	–0.001 ^{c)}	Δ_3 ^{d)}	1.6(3)
C(2)–C(3)	1.538(3) ^{e)}	C(2)–C(3)–C(4)	102.2(3) ^{e)}
C–C (ring)	1.539(3) ^{e)}	C(3)–C(4)–C(5)	111.5(3) ^{e)}
S–C(2)	1.826(4)	S–C(5)–C(4)	106.9(3) ^{e)}
C–H	1.129(3)	C(5)–S–C(2)	92.0(3) ^{e)}
Δ_2 ^{f)}	0.056(3)	C(2)–S=O	110.0(4) ^{e)}
S=O	1.484(3) ^{e)}	H–C–H	109.5 ^{e)}
		τ_2 ^{g)}	49.3(6)
		τ_5 ^{h)}	–13.3(13) ^{e)}
		τ_5/τ_2	–0.2706(260)
		ϕ ⁱ⁾	–60.6(7)



The nozzle temperature was 386 K.

^{a)} Estimated total errors.

^{b)} [C(2)–C(3)] – [C(3)–C(4)].

^{c)} Assumed.

^{d)} [S–C(5)–C(4)] – [S–C(2)–C(3)].

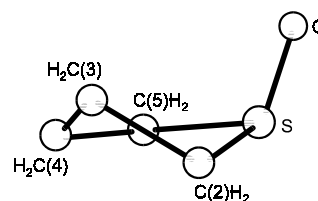
^{e)} Dependent parameter.

^{f)} [C(3)–C(4)] – (S=O).

^{g)} The puckering angle of the SC(2)C(3) plane with respect to the SC(3)C(4) plane.

^{h)} The puckering angle of the SC(5)C(4) plane with respect to the SC(3)C(4) plane.

ⁱ⁾ The angle between the C(5)SC(2) plane and the S=O bond.



Forgács, G., Schultz, G., Hargittai, I., Jalsovszky, I., Kucsman, A.: J. Chem. Soc., Faraday Trans. II **85** (1989) 303.

