

r_g	Å ^{a)}	θ_a	deg ^{a)}
S=O	1.437(3)	O=S–C(3)	105.2(5)
S–C (mean)	1.781(4)	O=S–C(4)	110.2(2)
C=C	1.344(5)	C–S–C	102.3(9)
C≡N	1.165(3)	S–C=C	114.9(6)
C(1)–C(2)	1.461 ^{b)}	C=C–C	121.5(7)
C–H (mean)	1.10 ^{b)}	O=S=O	121.4(7)
Δ(C–S) ^{c)}	0.015 ^{b)}	C(2)–C(1)≡N	179.7(19)
Δ(C–H) ^{d)}	0.01 ^{b)}	C=C–H	119.0 ^{b)}
		S–C–H	109(2)
		τ_1 ^{e)}	91(2)
		τ_2 ^{e)}	48(10)
		α_1 ^{f)}	0.85(4)

The molecule exists as a mixture of two conformers. The conformers were assumed to have the same geometry except for the torsional angle C–S–C=C.

The nozzle temperature was 384 K.

^{a)} Estimated total errors.

^{b)} Assumed.

^{c)} [C(4)–S] – [C(3)–S].

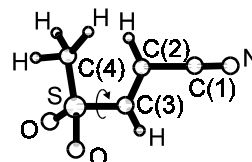
^{d)} [C(4)–H] – [C(2,3)–H].

^{e)} C–S–C=C torsional angles of the conformers I and II;

$\tau = 0^\circ$ for the *syn* position of the chain whose plane bisects the

O=S=O angle (see figure).

^{f)} Mole fraction of conformer I.



Vajda, E., Hnyk, D., Rozsondai, B., Podlaha, J., Podlahova, J., Hasek, J.: J. Mol. Struct. **239** (1990) 265.