

1605 C₄H₅NO₂S
ED

(Z)-3-(Methylsulfonyl)-2-propenenitrile

C₁ (*gauche*)
C₁ (*skew*)



r_g	Å ^{a)}	θ_a	deg ^{a)}
S=O	1.437(3)	O=S-C(3)	109.6(3)
S-C (mean)	1.780(4)	O=S-C(4)	104.3(3)
C=C	1.344(5)	C-S-C	108.4(5)
C≡N	1.168(3)	S-C=C	124.7(4)
C(1)-C(2)	1.435 ^{b)}	C=C-C	127.3(7)
C-H (mean)	1.115 ^{b)}	O=S=O	119.8(7)
Δ(C-S) ^{c)}	0.015 ^{b)}	C(2)-C(1)≡N	180 ^{b)}
Δ(C-H) ^{d)}	0.01 ^{b)}	C=C-H	118.2 ^{b)}
		S-C-H	109(2)
		τ ₁ ^{e)}	76(2)
		τ ₂ ^{e)}	111(4)
		α ₁ ^{f)}	0.68(4)

The molecule exists as a mixture of the *gauche* and *skew* conformers. The conformers were assumed to have the same geometry except for the torsional angle C-S-C=C.

The nozzle temperature was 375 K.

^{a)} Estimated total errors.

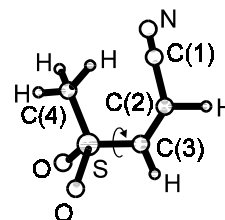
^{b)} Assumed.

^{c)} [C(4)-S] - [C(3)-S].

^{d)} [C(4)-H] - [C(2,3)-H].

^{e)} C-S-C=C torsional angles of the *gauche* and *skew* conformers;
τ = 0° for the *syn* position of the chain whose plane bisects the
O=S=O angle (see figure).

^{f)} Mole fraction of *gauche* conformer.



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