

1597
ED

C₄H₅NO

(Z)-3-Methoxy-2-propenenitrile
(Z)-3-Methoxyacrylonitrile

C₁ (*gauche*)
C₁ (*skew*)
H₃C–O–CH=CH–C≡N

r_g	Å ^{a)}	θ_a	deg ^{a)}
C–C	1.418(6)	O–C=C	120.8(9)
C=C	1.374(15)	C–O–C	117.9(9)
O–C (mean)	1.392(7)	C=C–C	126.1(7)
C≡N	1.161(3)	C=C–H	121 ^{b)}
C–H (mean)	1.100 ^{b)}	O–C–H	104(2)
$\Delta(\text{C–O})$ ^{c)}	0.085 ^{b)}	C–C≡N	180 ^{b)}
$\Delta(\text{C–H})$ ^{d)}	0.01 ^{b)}	τ_1 ^{e)}	56(3)
		τ_2 ^{e)}	133(3)
		α_1 ^{f)}	0.64(12)

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–O–C=C. The C(2)–C(1)≡N fragment is essentially linear. The nozzle temperature was 363 K.

^{a)} Estimated total errors.

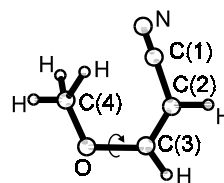
^{b)} Assumed. C–H (mean) corresponds to r_a .

^{c)} [C(4)–O] – [C(3)–O].

^{d)} [C(4)–H] – [C(2,3)–H].

^{e)} C–O–C=C torsional angles of the *gauche* and *skew* conformers; $\tau = 0^\circ$ for the *syn* position (see figure).

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



Hnyk, D., Vajda, E., Rozsondai, B.: J. Mol. Struct. **239** (1990) 281.