

1598
ED

C₄H₅NO

(*E*)-3-Methoxy-2-propenenitrile
(*E*)-3-Methoxyacrylonitrile

C_s (*syn*) assumed
C_s (*anti*) assumed
H₃C–O–CH=CH–C≡N

r_g	Å ^{a)}	θ_a	deg ^{a)}
C–C	1.428(5)	O–C=C	122.5(6)
C=C	1.348(8)	C–O–C	120.5(7)
O–C (mean)	1.393(6)	C=C–C	119.1(6)
C≡N	1.155(4)	C=C–H	120.0 ^{b)}
C–H (mean)	1.100 ^{b)}	O–C–H	107.3(5)
Δ(C–O) ^{c)}	0.095 ^{b)}	C–C≡N	180 ^{b)}
Δ(C–H) ^{d)}	0.01 ^{b)}	τ ₁ ^{e)}	0 ^{b)}
		τ ₂ ^{e)}	180 ^{b)}
		α ₁ ^{f)}	0.83(3)

The molecule exists as a mixture of the *syn* and *anti* 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 355 K.

^{a)} Estimated total errors.

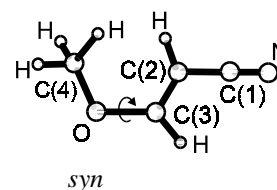
^{b)} Assumed. C–H (mean) corresponds to r_a .

^{c)} [C(4)–O] – [C(3)–O].

^{d)} [C(4)–H] – [C(2,3)–H].

^{e)} C–O–C=C torsional angles of the *syn* and *ant* conformers;
τ = 0° for the *syn* position (see figure).

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



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