

1601
MW

C₄H₅NO

3-Methylisoxazole

C_s

r_0	Å ^{a)}	θ_0	deg
C(5)=C(4)	1.362 ^{b)}	C(5)=C(4)–C(3)	102.7 ^{b)}
C(4)–C(3)	1.427 ^{b)}	C(4)–C(3)=N	112.5 ^{b)}
C(3)=N	1.310 ^{b)}	C(3)=N–O	105.2 ^{b)}
N–O	1.403 ^{b)}	N–O–C(5)	108.8 ^{b)}
O–C(5)	1.342 ^{b)}	O–C(5)=C(4)	110.7 ^{b)}
C(3)–C (I)	1.5272(50) ^{c)}	C–C(3)=N (I)	110.43 ^{b)} ^{c)}
C(3)–C (II)	1.5135(50) ^{c)}	C–C(3)=N (II)	118.8 ^{b)} ^{c)}

^{a)} Uncertainties were not estimated in the original paper.

^{b)} Assumed.

^{c)} The C(3)–C(methyl) bond was assumed to coincide with the CH₃ internal rotation axis. Their distances (I) and (II) were derived from assumptions for the angles (I) and (II), respectively.

Fliege, E.R.L.: Z. Naturforsch. **45a** (1990) 911.

