

1324
ED, MW

C₃H₇NO

(Z)-Propionaldehyde oxime

C_s (skeleton)
H₃C–CH₂–CH=NOH

r_g	Å ^{a)}	θ_α^0	deg ^{a)}
C(1)–C(2)	1.549(3)	C(1)–C(2)–C(3)	109.4(4)
C(2)–C(3)	1.497(2)	C(2)–C(3)=N	127.5(3)
C(3)=N	1.295(1)	C(3)=N–O	109.3(3)
N–O	1.430(2)	H–C(1)–H	111.8(8)
C(1)–H	1.125(2)	N–O–H	94.0(13)
$\Delta_1(\text{C–H})$ ^{b)}	0.009 ^{c)}	H–C(2)–H	109 ^{c)}
$\Delta_2(\text{C–H})$ ^{d)}	0.001 ^{c)}	N–C–H	114 ^{c)}
O–H	0.987(5)	tilt(CH ₃) ^{e)}	11.3(11)

The molecular skeleton is planar, but the internal rotation around the C(2)–C(3) bond is a large-amplitude motion. C_{3v} local symmetry of the CH₃ group was assumed.

The nozzle temperature was 26 °C.

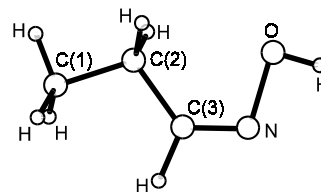
^{a)} Estimated limits of error.

^{b)} [C–H(methylene)] – [C–H(methyl)].

^{c)} Assumed according to *ab initio* calculations.

^{d)} [C–H(methyne)] – [C–H(methyl)].

^{e)} Tilt angle of the methyl group, away from the H atoms of the C(2)H₂ group.



Iijima, K., Ohashi, O.: J. Mol. Struct. **291** (1993) 159.

See also: (MW) Katayama, N., Sakaizumi, T., Yamaguchi, I., Ohashi, O.: Bull. Chem. Soc. Jpn. **59** (1986) 2911.