

1646
MW

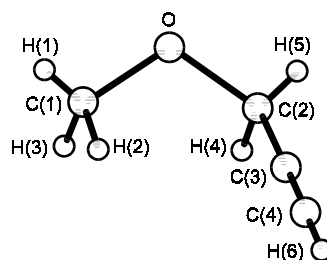
C₄H₆O

3-Methoxy-1-propyne
Methyl propargyl ether

C₁
H3C-O-CH2-C#CH

r_s	Å	θ_s	deg
C(3)≡C(4)	1.206 ^{a)}	C(2)–C(3)≡C(4)	180 ^{a)}
C(2)–C(3)	1.459 ^{a)}	C(3)–C(2)–O	112.5(20)
O–C(2)	1.410(20)	C–O–C	113.5(20)
O–C(1)	1.410(17)	H–C(4)≡C(3)	180 ^{a)}
C(4)–H(6)	1.056 ^{a)}	C(3)–C(2)–H(4)	108.7(20)
C(2)–H(4)	1.101 ^{a)}	C(3)–C(2)–H(5)	108.7(20)
C(2)–H(5)	1.101 ^{a)}	O–C(2)–H(4)	109.8 ^{a)}
C(1)–H(1)	1.078(19)	O–C(2)–H(5)	109.8 ^{a)}
C(1)–H(2)	1.170(9)	H(4)–C(2)–H(5)	107.2 ^{a)}
C(1)–H(3)	1.110(34)	O–C(1)–H(1)	107.4(17)
		O–C(1)–H(2)	109.9(15)
		O–C(1)–H(3)	109.9(20)
		H(1)–C(1)–H(2)	113.0(18)
		H(1)–C(1)–H(3)	108.9(27)
		H(2)–C(1)–H(3)	107.8(33)
		τ^b	67.5(20)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
O	1.1615	–0.3512	–0.4025
C(1)	1.5756	0.8699	0.1681
H(1)	2.4269	1.2163	–0.3953
H(2)	0.6865	1.6304	0.1676
H(3)	1.8844	0.7080	1.2219
C(2)	0.0453	–0.9229	0.2420
H(4)	0.2450	–1.0177	1.3206
H(5)	–0.1297	–1.9386	–0.1454
C(3)	–1.1692	–0.1356	0.0578
C(4)	–2.1730	0.5153	–0.0945
H(6)	–3.0520	1.0851	–0.2278



^{a)} Assumed.

^{b)} Dihedral angle C–C–O–C.

Hayashi, M., Nakagawa, J., Kato, H.: J. Mol. Spectrosc. **84** (1980) 362.

See also: Hayashi, M., Kato, H.: Bull. Chem. Soc. Jpn. **52** (1980) 2701.

Marstokk, K.M., Møllendal, H.: J. Mol. Struct. **32** (1976) 191.