

r_0	Å ^{a)}	θ_0	deg ^{a)}	
C(3)=C(4)	1.331 ^{b)}		conformer I	conformer II
C(2)–C(3)	1.496 ^{b)}	C–C–O	112.3 ^{b)}	
C(1)–C(2)	1.528 ^{b)}	C–O–H	105.0 ^{b)}	
C–O	1.415 ^{b)}	C=C–H	121.5 ^{b)}	
O–H	0.969 ^{b)}	H–C–H	109.5 ^{b)}	
C(1)–H	1.093 ^{b)}	C=C–C	126.8(20)	126.8(20)
C(2)–H	1.093 ^{b)}	C–C–C	110.3(20)	112.3(20)
C(3)–H	1.090 ^{b)}	α ^{c)}	122.0(20)	4.0(20)
C(4)–H	1.090 ^{b)}	β ^{d)}	53.0(20) ^{e)}	70.0(20) ^{f)}

The conformer I is more stable than II by 2.18(59) kJ mol^{−1}.

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

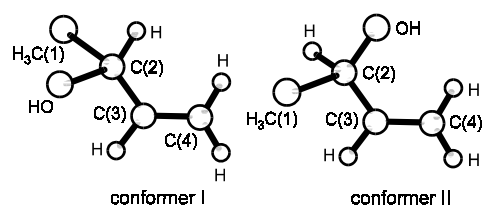
^{b)} Assumed.

^{c)} Dihedral angle O–C–C=C.

^{d)} Dihedral angle H–O–C(2)–C(3).

^{e)} Roughly *anti* to the methyl group.

^{f)} Roughly *anti* to the hydrogen on C(2).



Smith, Z., Carballo, N., Wilson, E.B., Marstokk, K.-M., Møllendal, H.: J. Am. Chem. Soc. **107** (1985) 1951.