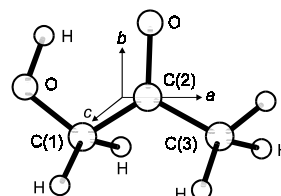


r_0	Å ^{a)}	θ_0	deg ^{a)}
C(1)–O	1.437 ^{b)}	C(1)–C(2)=O	122.7 ^{b)}
C(1)–C(2)	1.499 ^{b)}	C(2)–C(3)–H	109.3 ^{b)}
C(2)=O	1.216 ^{b)}	H–C(1)–H	107.6 ^{b)}
C(2)–C(3)	1.507 ^{b)}	H–C(1)–C(2)	109.2 ^{b)}
C(1)–H	1.093 ^{b)}	C(1)–O–H	103.6(10)
C(3)–H	1.085 ^{b)}	O–C(1)–C(2)	110.5(10)
O–H	1.051 ^{b)}	C(1)–C(2)–C(3)	117.6(10)

Atom	$a_s[\text{\AA}]$	$b_s[\text{\AA}]$	$c_s[\text{\AA}]$
H (hydroxyl)	-1.553	0.963	0.0



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

^{b)} Assumed.

Kattija-Ari, M., Harmony, M.D.: *Int. J. Quant. Chem.: Quant. Chem. Symp.* **14** (1980) 443.