

s-cis conformation

r_s	Å	θ_s	deg
C(1)–C(2)	1.479(2)	C(1)–C(2)=C(3)	121.4(1)
C(2)=C(3)	1.339(2)	O=C(1)–C(2)	124.3(1)
C(1)=O	1.213(2)	H(5)–C(1)–C(2)	115.5(2)
C(1)–H(5)	1.106(3)	C(3)=C(2)–H(6)	121.0(2)
C(2)–H(6)	1.087(3)	C(2)=C(3)–H(7)	118.5(2)
C(3)–H(7)	1.099(3)	C(2)=C(3)–H(8)	121.6(4)
C(3)–H(8)	1.081(1)	O=C(1)–H(5)	120.2(2)
		C(1)–C(2)–H(6)	117.6(2)
		H–C(3)–H	120.0(4)

r_0	Å	θ_0	deg
C(1)–C(2)	1.478(6)	C(1)–C(2)=C(3)	121.5(4)
C(2)=C(3)	1.340(7)	O=C(1)–C(2)	124.2(4)
C(1)=O	1.215(6)	H(5)–C(1)–C(2)	115.8(4)
C(1)–H(5)	1.106(4)	C(3)=C(2)–H(6)	121.1(4)
C(2)–H(6)	1.088(4)	C(2)=C(3)–H(7)	118.5(3)
C(3)–H(7)	1.098(5)	C(2)=C(3)–H(8)	121.5(6)
C(3)–H(8)	1.081(3)	O=C(1)–H(5)	120.1(4)
		C(1)–C(2)–H(6)	117.4(4)
		H–C(3)–H	120.0(5)

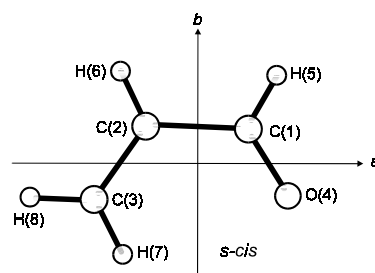
Atom	a_s [Å]	b_s [Å]	a_0 [Å]	b_0 [Å]
C(1)	0.7299	0.5173	0.7287	0.5202
C(2)	–0.7472	0.5911	–0.7473	0.5909
C(3)	–1.5014	–0.5154	–1.5013	–0.5165
O	1.3623	–0.5176	1.3624	–0.5162
H(5)	1.2554	1.4910	1.2564	1.4924
H(6)	–1.2014	1.5789	–1.2014	1.5793
H(7)	–0.9985	–1.4922	–0.9988	–1.4925
H(8)	–2.5813	–0.4643	–2.5812	–0.4659

s-trans conformation

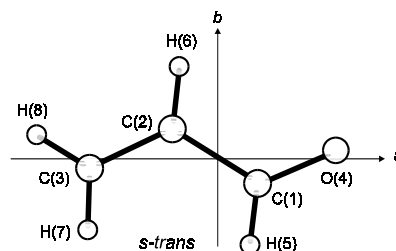
r_s	Å	θ_s	deg
C(1)–C(2)	1.468(3)	C(1)–C(2)=C(3)	120.3(4)
C(2)=C(3)	1.341(5)	O=C(1)–C(2)	123.9(3)
C(1)=O	1.215(3)	H(5)–C(1)–C(2)	114.7(4)
C(1)–H(5)	1.113(3)	C(3)=C(2)–H(6)	122.4(5)
C(2)–H(6)	1.084(4)	C(2)=C(3)–H(7)	119.8(4)
C(3)–H(7)	1.089(10)	C(2)=C(3)–H(8)	122.2(9)
C(3)–H(8)	1.081(7)	O=C(1)–H(5)	121.3(5)
		C(1)–C(2)–H(6)	117.3(4)
		H–C(3)–H	118.0(5)

r_0	Å	θ_0	deg
C(1)–C(2)	1.468(4)	C(1)–C(2)=C(3)	120.4(5)
C(2)=C(3)	1.340(4)	O=C(1)–C(2)	124.0(6)
C(1)=O	1.214(4)	H(5)–C(1)–C(2)	114.7(5)
C(1)–H(5)	1.113(6)	C(3)=C(2)–H(6)	122.4(4)
C(2)–H(6)	1.084(5)	C(2)=C(3)–H(7)	119.7(3)
C(3)–H(7)	1.090(4)	C(2)=C(3)–H(8)	122.2(5)
C(3)–H(8)	1.080(3)	O=C(1)–H(5)	121.3(6)
		C(1)–C(2)–H(6)	117.2(5)
		H–C(3)–H	118.1(6)

Atom	a_s [Å]	b_s [Å]	a_0 [Å]	b_0 [Å]
C(1)	0.5908	-0.3646	0.5910	-0.3643
C(2)	-0.6356	0.4422	-0.6353	0.4422
C(3)	-1.8372	-0.1523	-1.8372	-0.1508
O	1.7112	0.1048	1.7113	0.1034
H(5)	0.4243	-1.4649	0.4243	-1.4649
H(6)	-0.5215	1.5205	-0.5200	1.5197
H(7)	-1.9029	-1.2392	-1.9026	-1.2386
H(8)	-2.7584	0.4124	-2.7586	0.4136



Blom, C. E., Grassi, G., Bauder, A.: J. Am Chem. Soc. **106** (1984) 7427.



ED, MW

s-trans conformation

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(1)–C(2)	1.484(4)	C(1)–C(2)=C(3)	120.3(7)
C(2)=C(3)	1.345(3)	O=C(1)–C(2)	123.3(7)
C(1)=O	1.217(3)	H(5)–C(1)–C(2)	114.4(27)
C(3)–H(7,8)	1.100(10)	C(3)=C(2)–H(6)	122.9(18)
C(1)–H	1.128(30)	C(2)=C(3)–H(8)	121.5(11)
		C(2)=C(3)–H(7)	119.6(11)

The molecule is assumed to be planar. The above data are based on the experimental results of Ref.[1].

The measurements were made at room temperature.

^{a)} Estimated limits of error.

Kuchitsu, K., Fukuyama, T., Morino, Y.: J. Mol. Struct. **4** (1969) 41.

[1] Kuchitsu, K., Fukuyama, T., Morino, Y.: J. Mol. Struct. **1** (1968) 463.

See also: Trætteberg, M.: Acta Chem. Scand. **24** (1970) 373.

UV

s-trans conformation

State		\tilde{A}^1A''
Energy [eV]		3.206
r_0 [Å]	C(1)–C(2)	1.46
	C(2)=C(3)	1.35
	C(1)=O	1.32
	C–H	1.09
θ_0 [deg]	C(1)–C(2)=C(3)	125
	C(2)–C(1)=O	125
	C–C–H	120

Rotational and vibrational analysis.

These dimensions are consistent with limited inertial information from rotational analysis, but are by no means unique.

Hollas, J.M.: Spectrochim. Acta **19** (1963) 1425.