

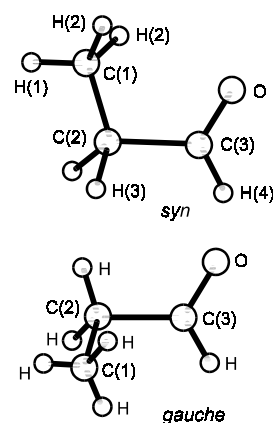
r_s	\AA		θ_s	deg	
	<i>syn</i>	<i>gauche</i>		<i>syn</i>	<i>gauche</i>
C(1)–C(2)	1.523(4)	1.519(9)	H(1)–C(1)–H(2)	108.7(4)	
C(1)–H(2)	1.103(2)		H(2)–C(1)–C(2)	110.3(2)	
C(1)–H(1)	1.096(3)		H(2)–C(1)–H(2)	107.0(3)	
C(2)–H	1.105(2)		H–C(2)–C(3)	111.9(2)	
C(2)–C(3)	1.509(4)	1.509(9)	C–C–C	113.8(2)	111.7(4)
C(3)=O	1.210(4)		H–C(2)–H	105.0(5)	
C(3)–H	1.115(3)		C(2)–C(3)=O	124.4(2)	125.1(9)
			C(2)–C(3)–H	115.1(2)	
			$\tau(\text{C–C–C=O})$	0 ^{a)}	128.2(3)

syn conformer

Atom	a_s [\AA]	b_s [\AA]	c_s [\AA]
C(1)	–1.4858	0.5658	
C(2)	–0.6737	–0.7226	
C(3)	0.8185	–0.5009	
H(1)	–2.5637	0.3666	
H(2)	–1.2380	1.1744	± 0.8864
H(3)	–0.9097	–1.3547	± 0.8755
O	1.3474	0.5870	
H(4)	1.4348	–1.4306	

gauche conformer

Atom in CHO group	a_s [\AA]	b_s [\AA]	c_s [\AA]
O	–1.7154	–0.0292	–0.2422
H	–0.5817	–0.9993	1.1182

^{a)} By symmetry.

Randell, J., Cox, A.P., Hillig, K.W., Imachi, M., LaBarge, M.S., Kuczkowski, R.L.: Z. Naturforsch. **43a** (1988) 271.

ED

r_g	\AA ^{a)}	θ_α	deg ^{a)}
C(1)–C(2)	1.549(8)	C(2)–C(1)–H	110.7(16)
C(2)–C(3)	1.497(8)	C(3)–C(2)–H	110.2 ^{b)}
C(3)=O	1.215(3)	C–C–C	113.3(3)
C–H	1.110(6)	C(2)–C(3)=O	125.7(5)
C–C(average)	1.523(4)	C(2)–C(3)–H	114.0 ^{b)}
		$\tau(\text{C–C–C=O})$	126(16) ^{c)}
		ϕ ^{d)}	60.0 ^{b)}

A mixture of conformers with C(3)=O and C(2)–C(3) *syn* (65(12)%) and *gauche* to each other were observed.

By combination with the ED data reported in [1], where the amount of the *gauche* conformer was 19(3)%, $\Delta E = E(\textit{gauche}) - E(\textit{syn}) = 1.5$ ($\sigma = 0.7$) kcal mol^{–1} and $\Delta S = S(\textit{gauche}) - S(\textit{syn}) = 0.6$ ($\sigma = 2$) cal mol^{–1} K^{–1} were obtained.

The nozzle temperature was 448 K.

^{a)} Three times the estimated standard errors.^{b)} Assumed.^{c)} Torsion angle for *gauche* conformer, $\tau = 0^\circ$ for the *syn* position.^{d)} Angle of CH₃ torsion measured from the eclipsed position (undefined in the original paper).

Skjørholm, S.J., Hagen, K.: J. Mol. Struct. **156** (1987) 155.

[1] van Nuffel, P., van den Enden, L., van Alsenoy, C., Geise, H.J.: J. Mol. Struct. **116** (1984) 99.