

1275
MW

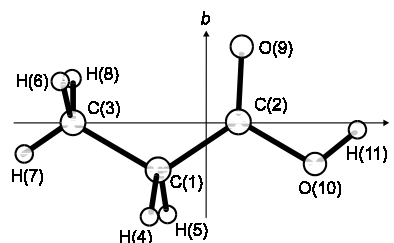
C₃H₆O₂

Propionic acid

C_s (syn)
H₃C–CH₂–C(O)–OH

r_s	Å	θ_s	deg
C(1)–C(2)	1.509(2)	C(3)–C(1)–C(2)	112.7(1)
C(1)–C(3)	1.523(3)	C(2)–C(1)–H(4,5)	107.7(2)
C(1)–H(4,5)	1.098(2)	H(4)–C(1)–H(5)	106.4(2)
C(3)–H(6,8)	1.087(2)	H(6)–C(3)–H(8)	108.5(1)
C(3)–H(7)	1.088(2)	C(1)–C(3)–H(6,8)	110.3(2)
C(2)=O(9)	1.210(1)	H(6,8)–C(3)–H(7)	108.8(1)
C(2)–O(10)	1.352(2)	C(1)–C(3)–H(7)	109.8(3)
O(10)–H(11)	0.970(1)	C(1)–C(2)=O(9)	125.8(2)
O(9)...O(10)	2.245(1)	C(1)–C(2)–O(10)	111.8(1)
		C(2)–O(10)–H(11)	105.8(2)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(1)	–0.7644	–0.7708	0.0
C(2)	0.4842	0.0765	0.0
C(3)	–2.0408	0.0623	0.0
H(4,5)	–0.7036	–1.4248	±0.8792
H(6,8)	–2.0790	0.6957	±0.8822
H(7)	–2.9082	–0.5927	0.0
O(9)	0.5220	1.2863	0.0
O(10)	1.6053	–0.6796	0.0
H(11)	2.3452	–0.0520	0.0



Stiefvater, O.L.: J. Chem. Phys. **62** (1975) 244.

ED

C_s (syn)
C₁ (nonplanar)

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(1)–C(2)	1.515(30)	C(3)–C(1)–C(2)	112.8(30)
C(1)–C(3)	1.540(30)	C(1)–C(2)=O(9)	126.7(24)
C–H	1.123(40)	C(1)–C(2)–O(10)	111.2(24)
C(2)=O(9)	1.209(9)		
C(2)–O(10)	1.364(12)		

At 55(5) °C molecule exists as a mixture of the monomer (about 48 mol%) and dimer (about 52 mol%). At 215(10) °C the experimental data are consistent with only the monomer being present as a mixture of two conformers, one with the C(1)–C(3) bond eclipsed with respect to the C(2)=O(9) bond and the other with a nonplanar skeleton.

^{a)} Estimated standard errors, three times those in the original paper.

Derissen, J.L.: J. Mol. Struct. **7** (1971) 81.