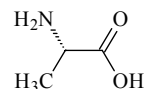
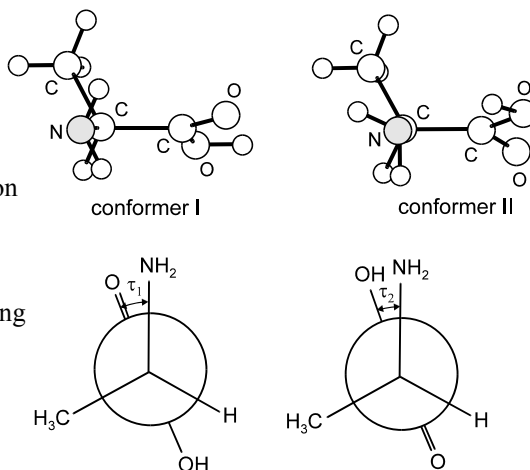


434 **C₃H₇NO₂**ED, MW, *ab initio*
calculations**L-Alanine** α -Alanine**C₁** (conformer I)**C₁** (conformer II)

r_{α}^0	\AA^a		θ_{α}^0	deg^a	
	I	II		I	II
C–C (average)	1.531(1)	1.535	C–C=O	125.7(3)	122.9
C=O	1.197(1)	1.194	C–C–O	110.3(2)	112.9
C–O	1.341(2)	1.327	C–C–C(methyl)	111.9(2)	111.7
C–N	1.453(2)	1.469	N–C–C	112.9(3)	108.6
C–H (average)	1.050(4)	1.051	N–C–C(methyl)	110.0(2)	112.5(4)
C–C ^{b)}	1.527	1.538	τ_1^c	–16.6(4)	
C–C(methyl) ^{b)}	1.536	1.532	τ_2^d		–16.9(4)

In contradiction to a previous study [1], it was found that the molecule exists as a mixture of two conformers. It was confirmed that the molecule takes a neutral form in the gas phase. The main species (89(4)%) has the conformation with $\text{NH}_2 \dots \text{O}=\text{C}$ hydrogen bonding, while the minor species (11(4)%) has the conformation with $\text{H}_2\text{N} \dots \text{HO}$ hydrogen bonding. Differences between corresponding parameters of these conformers except for N–C–C(methyl) bond angles and torsional angles were assumed at the values from MP2/6-311++G** calculations [2]. The sample was vaporized at *ca.* 230 °C.



^{a)} 2.6 times the estimated standard errors including a systematic error.

^{b)} Difference between the C–C(methyl) and C–C bond lengths were assumed at the value from MP2/6-311++G** calculations [2].

^{c)} Torsional angle N–C–C=O, $\tau_1 = 0^\circ$ for the *syn* position.

^{d)} Torsional angle N–C–C–O(H), $\tau_2 = 0^\circ$ for the *syn* position.

Iijima, K., Nakano, M.: J.Mol. Struct. **485-486** (1999) 255.

[1] Iijima, K., Beagley, B.: J. Mol. Struct. **248** (1991) 133.

[2] Császár, A.G.: J. Phys. Chem. **100** (1996) 3541.

Replaces [II/25C \(3, 1331\)](#)