

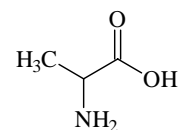
1331  
ED

**C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>**

**L-Alanine**

**C<sub>1</sub>**

| $r_g$      | Å <sup>a)</sup> | $\theta_\alpha$        | deg <sup>a)</sup>       |
|------------|-----------------|------------------------|-------------------------|
| C–N        | 1.471(7)        | N–C(2)–C(1)            | 110.1(8)                |
| C(1)–C(2)  | 1.544(10)       | N–C(2)–C(3)            | 110.0(16) <sup>b)</sup> |
| C–C (mean) | 1.526(4)        | C(2)–C(1)=O(1)         | 125.6(7)                |
| C=O(1)     | 1.192(2)        | C(2)–C(1)–O(2)         | 110.3(7)                |
| C–O(2)     | 1.347(3)        | C(1)–C(2)–C(3)         | 111.6(11)               |
| C–C(m)     | 1.509(16)       | $\tau_1$ <sup>c)</sup> | 123.8(17)               |
|            |                 | $\tau_2$ <sup>d)</sup> | 17(2)                   |



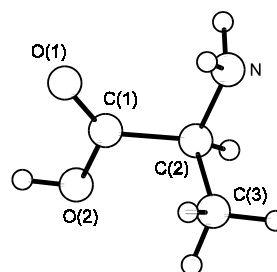
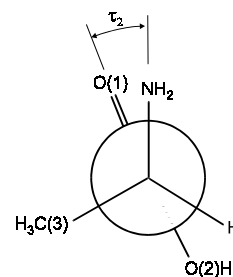
Only one conformer of a neutral species was observed in the vapor phase. The CCOOH group was assumed to be planar. The nozzle temperature was 513 K.

<sup>a)</sup> Estimated limits of error.

<sup>b)</sup> Dependent parameter.

<sup>c)</sup> Dihedral angle between the NC(2)C(1) plane and the C(3)C(2)C(1) plane.

<sup>d)</sup> Dihedral angle between the NC(2)C(1) plane and the C(2)C(1)O(1) plane. The distortion is in the direction shown in the figure.



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