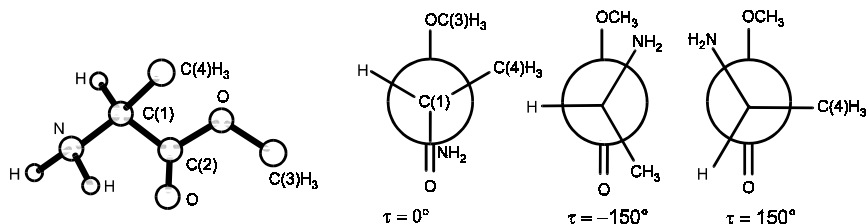
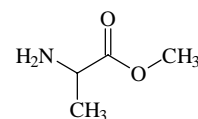


ED, *ab initio* calculations
(HF/4-21G)

r_g	Å	θ_e °	deg
C(2)=O	1.208(4)	N-C(1)-C(4)	110.19
C(1)-C(2)	1.518(8) ^{b)}	N-C(1)-C(2)	111.90
C(1)-N	1.457(8) ^{b)}	C(1)-C(2)=O	126.12
C(2)-O	1.353(8) ^{b)}	C(1)-C(2)-O	111.14
O-C(3)	1.455(8) ^{b)}	C(2)-O-C(3)	117.74
C(1)-C(4)	1.536(8) ^{b)}	C(4)-C(1)-C(2)	109.88
		C(4)-C(1)-C(2)-O	61.4



The ED data were consistent with a model for the most populated conformational state in which the N-C-C=O torsion is *synperiplanar* ($\tau = 0^\circ$) and a bifurcated hydrogen bond exists between NH₂ and C=O. The presence of a significant concentration of a second conformer, ($\tau \approx +150^\circ$), could not be ruled out, whereas the *ab initio* calculations predicted greater stability of a conformer with $\tau \approx -150^\circ$ than $+150^\circ$. No clear-cut conclusion has yet been reached on this problem. The calculations indicate that the C(1), C(2), =O, -O and C(3) atoms are essentially coplanar (O=C(2)-O-C(3) being *synperiplanar*) in these conformers.

The nozzle temperature was $\approx 80^\circ\text{C}$.

^{a)} Three times the estimated standard errors.

^{b)} The differences in these bond lengths were assumed to be those estimated by the *ab initio* calculations.

^{c)} For the *syn* conformer ($\tau = 0^\circ$), estimated by the *ab initio* calculations.

Ewbank, J.D., Klimkowski, V.J., Siam, K., Schäfer, L.: J. Mol. Struct. **160** (1987) 275.