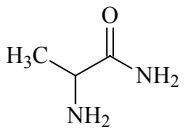
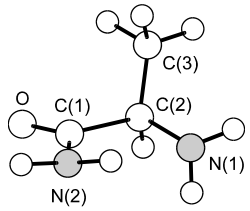
440 **$C_3H_8N_2O$** **Alaninamide** **C_1**
MW
Alanine amide
2-Aminopropanamide



r_0	Å	θ_0	deg
N(1)–C(2)	1.482(6)	N(1)–C(2)–C(3)	109.7(2)
C(2)–C(1)	1.528(8)	N(1)–C(2)–C(1)	109.3(16)
C(2)–C(3)	1.520(5)	C(2)–C(1)=O	119.0(26)
C(1)=O	1.258(30)	C(2)–C(1)–N(2)	117.2(18)
C(1)–N(2)	1.331(36)	N(1)–C(2)–C(1)–N(2) [a])	21.0(30) [b])
		N(1)–C(2)–C(1)=O [a])	–167.4(30) [b])
		C(3)–C(2)–C(1)–N(2) [a])	–100.0(30) [b])

Atom	a_0 [Å]	b_0 [Å]	c_0 [Å]
N(1)	1.455	–1.042	0.307
H [N(1)]	2.450	–0.837	0.344
H [N(1)]	1.258	–1.604	1.131
C(2)	0.701	0.232	0.392
H [C(2)]	0.719	0.695	1.392
C(3)	1.266	1.228	–0.607
H [C(3)]	0.664	2.141	–0.599
H [C(3)]	2.301	1.487	–0.357
H [C(3)]	1.248	0.796	–1.614
C(1)	–0.778	–0.036	0.119
O	–1.618	0.864	0.377
N(2)	–1.083	–1.150	–0.542
H [N(2)]	–0.319	–1.723	–0.870
H [N(2)]	–1.982	–1.187	–0.996



The observed spectra can be assigned to a conformation with an intramolecular hydrogen bond from the amide to the amine.

[a]) Dihedral angle.
[b]) Uncertainties were not estimated in the original paper.

Lavrich, R.J., Farrar, J.O., Tubergen, M.J.: J. Phys. Chem. A **103** (1999) 4659.