

Structure Data of Free Polyatomic Molecules

 457
MW

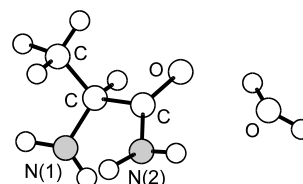
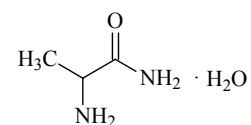
 $\text{C}_3\text{H}_7\text{N}_2\text{O}_2$
Alaninamide – water (1/1)
(weakly bound complex)

 C_1

(large-amplitude motion)

r_0	\AA
$r_1^{\text{a)}}$	2.042(6)
$r_2^{\text{b)}}$	1.931(4)

Atom	$ a_s [\text{\AA}]$	$ b_s [\text{\AA}]$	$ c_s [\text{\AA}]$
N(1)	2.096	1.095	0.12
N(2)	0.481	1.095	0.399


^{a)} The intermolecular hydrogen bond length (amide to water).

^{b)} The intermolecular hydrogen bond length (water to carbonyl).

 Lavrich, R.J., Tubergen, M.J.: J. Am. Chem. Soc. **122** (2000) 2938.