

Structure Data of Free Polyatomic Molecules

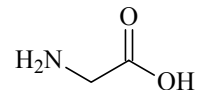
 286
MW

 $\text{C}_2\text{H}_5\text{NO}_2$

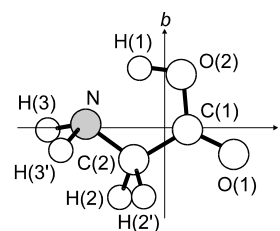
Glycine

 C_s assumed
(effective symmetry class)

r_0	\AA^{a}	θ_0	deg^{a}
O–H	0.98(2)	C–O–H	105(1)
N–H	1.01(2)	C–N–H	113(7)
C–H	1.10(2)	N–C–H	112(1)
C=O(1)	1.21(2)	C–C=O(1)	122(4)
C–O(2)	1.33(4)	C–C–O(2)	115(2)
C–C	1.52(3)	C–C–N	112(2)
N–C	1.46(3)	H–C–H	107(2)
		H–N–H	110(3)



Atom	a_0 [\AA]	b_0 [\AA]	c_0 [\AA]
H(1)	−0.5021	1.4305	0.0
O(2)	0.4638	1.2845	0.0
C(1)	0.6016	−0.0403	0.0
O(1)	1.6757	−0.5957	0.0
C(2)	−0.7066	−0.8228	0.0
H(2,2')	−0.6903	−1.4719	± 0.8849
N	−1.8680	0.0673	0.0
H(3,3')	−2.4342	−0.0384	± 0.8243



The structure of the conformer that has the strongest microwave spectrum is listed.

^a) Estimated standard errors.

McGlone, S.J., Elmes, P.S., Brown, R.D., Godfrey, P.D.: J. Mol. Struct. **485-486** (1999) 225.

[II/25B\(3, 835\)](#)