

Species Tag:	75003	Name:	H2NCH2COOH II
Version:	1		Glycine, Conformer II
Date:	Jan. 1996		ground and first
Contributor:	H. S. P. Müller		excited torsional states

Lines Listed:	26544	Q(300.0)=	124879.8881
Freq. (GHz) <	1000	Q(225.0)=	100530.4504
Max. J:	40	Q(150.0)=	68673.2239
LOGSTR0=	-11.0	Q(75.00)=	29376.5224
LOGSTR1=	-8.0	Q(37.50)=	10752.5529
Isotope Corr.:		Q(18.75)=	3810.1565
Egy. (cm ⁻¹) >	700.0	Q(9.375)=	1350.3826
μ_a =	5.372	A=	10130.152
μ_b =	0.930	B=	4071.5075
μ_c =		C=	3007.4892

This conformer of glycine is ≈ 700 cm⁻¹ higher in energy than conformer I (2, 3). The data were taken from (1) R. D. Suenram and F. J. Lovas, 1978, *J. Mol. Spectrosc.* **72**, 372 (millimeterwave region), and (2) F. J. Lovas, Y. Kawashima, J.-U. Grabow, R. D. Suenram, G. T. Fraser, and E. Hirota, 1995, *Astrophys. J. Lett.* **455**, 201; (microwave region, dipole moment, and ¹⁴N quadrupole coupling).

The ground and first excited states have been fit simultaneously, using only changes in the vibrational constants and D_{JK} for the excited state. The estimated torsional energy of 87 cm⁻¹ has been taken from an *ab initio* calculation (SCF/DZP, scaled by 0.9; (3) C. H. Hu, M. Shen, and H. F. Schaefer, III, 1993, *J. Am. Chem. Soc.* **115**, 2923).

For low J (< 10) hyperfine splittings are included in the catalog.

For the relative intensities between ground and first excited torsional states the approximate position of the torsional state was taken into account. Because there are several low lying vibrational modes that have not been investigated, the partition function was calculated for the ground state of the lower energy conformation including the nitrogen spin degeneracy. The partition function was calculated up to $J = 150$ because of the small rotational constants.