Species Tag:	75002	Name:	H2NCH2COOH I
Version:	1		Glycine, Conformer I
Date:	Jan. 1996		ground and first
Contributor:	H. S. P. Müller		excited torsional states

Lines Listed:	27217	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}) >	0.0	Q(9.375)=	1350.3826
$\mu_a =$	0.911	A=	10341.530
$\mu_b =$	0.607	B=	3876.1798
$\mu_c =$		C=	2912.3525

This is the lowest energy conformer of glycine. The data were taken from (1) R. D. Suenram and F. J. Lovas, 1980, J. Am. Chem. Soc. **102**, 7180 (millimeter wave 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 ^{14}N quadrupole coupling).

The ground and first excited states have been fit simultaneously, using only changes in the vibrational constants for the excited state. The reported hyperfine splittings have been used in the fit, but because they were well below 1 MHz for the strongest lines, they have not been included in the catalog file. The estimated torsional energy of 72 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).

In (1) lines were also reported for the second and third excited torsional state.

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 investgated, the partition function was calculated for the ground state alone, including the nitrogen spin degeneracy. The partition function was calculated up to $J = 150$ because of the small rotational constants.