Species Tag:	75004		Name:	H2NCO2CH3
Version:	1			Methyl Carbamate,
Date:	May 2009			$v_T = 0,1$
Contributor:	B.J. Drouin			A, E states

Lines Listed:	140822		Q(300.0)=	1321042.0
Freq. (GHz) <	1000		Q(225.0)=	812741.1
Max. J:	50		Q(150.0)=	398491.5
LOGSTR0=	-9.0		Q(75.00)=	118060.2
LOGSTR1=	-7.0		Q(37.50)=	38350.6
Isotope Corr.:	0.0		Q(18.75)=	13435.5
Egy. (cm^{-1}) >	0.0		Q(9.375)=	4758.1
$\mu_a =$	0.163		A=	9963.90
$\mu_b =$	2.294		B=	5161.94
$\mu_c =$			C=	3184.78

The data set used is from V. Ilyushin, E. Alekseev, J. Demaison, I. Kleiner, J. Mol. Spectrosc. 240 (2006) 127-132 and includes data from
K.-M.Marstokk, H. Mollendal, Acta Chem. Scand. 53 (1999) 79-84.
B. Bakri, J. Demaison, I. Kleiner, L. Margules, H. Mollendal, D. Petitprez, G. Wlodarczak, J. Mol. Spectros. 215 (2002) 312-316.

An internal rotor Hamiltonian, based on the "ρ axis method", similar to that developed for this species by Ilyushin *et al.*, was utilized for fitting of the torsion-rotation spectrum. A primary difference in the analysis regards the usage of the internal rotation operator, p, in IAMCALC/SPFIT the operator always appears as $\tilde{p}$ $= p + \rho P_a$ whereas Kleiner's program uses this combination only in the definition of F and simply uses p in all other operator definitions. The program IAMCALC utilises the Mathieu function to generate an extensive set of linked parameters that connect torsional levels ($v_T = 0$-1, A, E) defined as per the table below. Additional levels up to $v = 20$ ($v_T = 6$) were utilized for the basis set, these levels do not accurately describe higher torsional levels due to their position near or above the barrier to internal rotation, therefore predictions are truncated at the 1st torsional level. The dipole moment components specified in the '.int' file are given in the ρ axis system and are equivalent to principle axes values upon rotation. The rotational constants given here have been rotated from the ρ axis system using D_{ab} to obtain principle axis values. The data analysis extends to $J = 20$ and fits data to experimental precision. The calculation is extended to $J = 50$. The partition function was determined for the torsion-rotation problem in a separate calculation in which the maximum J was extended to 109. This partition function was multiplied by 3 to account for the effect of the hyperfine splittings used in the final fit and prediction. Note that this partition function implicitly includes the ground and first torsional levels, thus representing a partial vibrational partition function.

The analysis was performed on primarily hyperfine removed data, with the exeption of the FTMW data set. Predictions include full hyperfine splittings and therefore much of the data set is not merged in the catalog.

The dipole moments are from K.-M.Marstokk, H. Mollendal, Acta Chem. Scand. 53 (1999) 79-84.

	gs	$v_T = 1$	
A	0	3	
E	1,2	4,5	