

Species Tag:	44003	Name:	CH3CHO
Version:	3		Acetaldehyde
Date:	Jan. 2012		ground, 1 st and 2 nd torsional states,
Contributor:	H. M. Pickett		A & E species
	B. J. Drouin		
Lines Listed:	47034	Q(300.0)=	86841.0823
Freq. (GHz) <	900	Q(225.0)=	50049.7231
Max. J:	46	Q(150.0)=	22892.2045
LOGSTR0=	-9.5	Q(75.00)=	6495.8039
LOGSTR1=	-9.0	Q(37.50)=	2154.5221
Isotope Corr.:	0.	Q(18.75)=	760.2458
Egy. (cm ⁻¹) >	0.0	Q(9.375)=	270.1167
μ_a =	2.4234	A=	56507.198
μ_b =	-1.260	B=	10454.077
μ_c =		C=	9089.087

The data, including combination difference energy levels were taken from Kleiner, Lovas & Godefroid, *J. Phys. Chem. Ref. Data*, Vol 25, No. 4, 1996, and references therein. An internal rotor Hamiltonian, based on the “ ρ axis method”, similar to that developed for this species by Hougen and Kleiner, was utilized for fitting of the torsion-rotation spectrum. A primary difference in the analysis include the usage of the internal rotation operator, p , in IAMCALC/SPFIT the operator always appears as $\tilde{p} = p + \rho P_a$ whereas Kleiner 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 sublevels ($v_T = 0-2$, 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 above the barrier to internal rotation, therefore predictions are truncated at the 2nd torsional level. The dipole moment components are given in the ρ axis system and are processed by IAMCALC. The rotational constants given here are also in the ρ axis system and must be diagonalized with $D_{ab} = -3677.76$ to obtain principle axis values. The data analysis extends to $J = 26$ and fits data to experimental precision, however much of the frequency data above 300 GHz is of 1 MHz precision or worse. The calculation is extended to $J = 46$ at which point energy level uncertainties approach 1 cm⁻¹. The frequency cutoff is chosen to coincide with the $J = 46$ R-branch. The partition function was determined in a separate calculation in which the maximum J was extended to 86. Between $J = 66$ and $J = 86$ the 300 K partition sum grew only 1% and the 225 K sum grew by only 0.01%, all lower temperature were unchanged, indicating good convergence. Note that this partition function implicitly includes the ground and first two torsional levels, thus representing a partial vibrational partition function.

	gs	$v_T = 1$	$v_T = 2$
A	0	3	6
E	1,2	4,5	7,8

Version 3 is simply a re-prediction of the version 2 catalog with lower intensity thresholds and transitions with redundant quanta have been merged.